

=> d his

(FILE 'HOME' ENTERED AT 15:01:19 ON 26 OCT 2003)

FILE 'MEDLINE, CAPLUS, BIOSIS, EMBASE, SCISEARCH, AGRICOLA'  
ENTERED AT

15:01:49 ON 26 OCT 2003

L1 59314 S VANCOMYCIN  
L2 11148 S THIOESTER  
L3 8 S L1 (P) L2  
L4 4 DUPLICATE REMOVE L3 (4 DUPLICATES REMOVED)  
L5 208123 S BACTERIA? (P) DISEASE  
L6 0 S L4 (P) L5  
L7 945 S L1 (P) L5  
L8 1668953 S IN VIVO  
L9 1 S L4 (P) L8  
L10 32 S MU YONGQI/AU  
L11 1 S L10 AND L4  
L12 0 S L11 NOT L9  
L13 5 S L10 AND L1  
L14 5 DUPLICATE REMOVE L13 (0 DUPLICATES REMOVED)  
L15 4 S L14 NOT (L9 OR L4)

=> log y

	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments	Error Definition	Errors
1	BRS	L1	7	mu adj yongqi.in.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/10/26 13:25			0
2	BRS	L3	9174	thioester	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/10/26 13:26			0
3	BRS	L4	1	2 same 3	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/10/26 13:26			0
4	BRS	L2	73	A82846B or chloroorienticin or LY264826	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/10/26 13:28			0

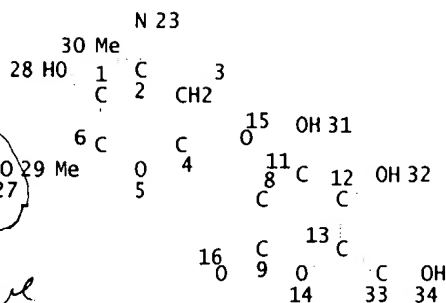
NO cpds fit the claimed sth  
in Beilstein

KAM 09/847,048

=> d que 127  
L13

STR

parent cpd sth



must be  
attached  
somewhere

ring  
only

ring only bonds

NODE ATTRIBUTES:

CONNECT IS M2 RC AT 23

CONNECT IS E2 RC AT 25

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

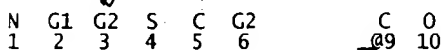
L25 65 SEA FILE=BEILSTEIN SSS FUL L13

L26 AK1 STR

subset str

65 cpds

CB uHy 11  
O



cpd must have this moiety

REP G1=(0-1) 9

VAR G2=AK/CB/HY

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L27 0 SEA FILE=BEILSTEIN SUB=L25 SSS FUL L26

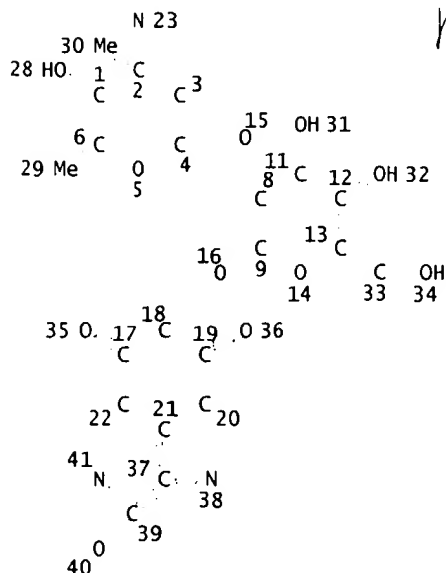
no cpds

~~Bel~~ no cpts fit claimed  
str in Reg

KAM 09/847,048

=> d que 128

L11 3000 SEA FILE=REGISTRY ABB=ON PLU=ON 23290.1.1/RID AND 46.157.1/R  
ID  
L12 517 SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND S/ELS  
L16 STR



NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE  
L19 377 SEA FILE=REGISTRY SUB=L12 SSS FUL L16  
L21 STR 1st subset

S C 0  
1 2 3 ← must be in str somewhere

NODE ATTRIBUTES:  
CONNECT IS E2 RC AT 1  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE  
L23 45 SEA FILE=REGISTRY SUB=L19 SSS FUL L21  
L26 STR

11  
0 2nd subset - further refinement

N G1 G2 S C G2 C O  
1 2 3 4 5 6 @9 10

REP G1=(0-1) 9  
VAR G2=AK/CB/HY  
NODE ATTRIBUTES:

KAM 09/847,048

DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE  
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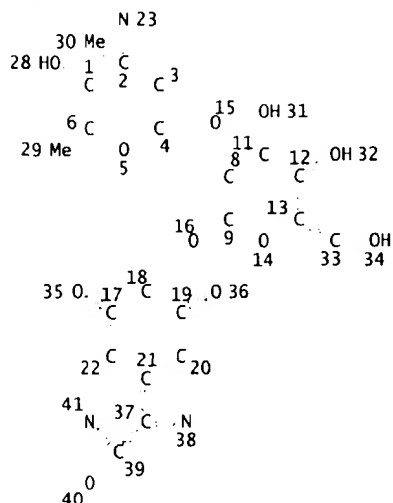
*no cys*

=&gt; d que 124

L11 3000 SEA FILE=REGISTRY ABB=ON PLU=ON 23290.1.1/RID AND 46.157.1/R

L12 517 SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND S/ELS

L16 STR



These are refs  
that have a s-c  
group but don't  
fit the claimed  
STR.

NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE  
L19 377 SEA FILE=REGISTRY SUB=L12 SSS FUL L16  
L21 STR

S C 0  
1 2 3

NODE ATTRIBUTES:  
CONNECT IS E2 RC AT 1  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE  
L23 45 SEA FILE=REGISTRY SUB=L19 SSS FUL L21  
L24 3 SEA FILE=CAPLUS ABB=ON PLU=ON L23

45 cpds  
3 cites

=&gt; d ibib abs hitstr 124 1-3

L24 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:689112 CAPLUS

DOCUMENT NUMBER: 136:70060

TITLE: Synthesis and biological evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria: target-accelerated combinatorial synthesis

AUTHOR(S): Nicolaou, K. C.; Hughes, Robert; Cho, Suk Young; Winssinger, Nicolas; Labischinski, Harald; Endermann, Rainer

CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Chemistry--A European Journal (2001), 7(17), 3824-3843  
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Based on the notion that dimerization and/or variation of amino acid 1 of vancomycin could potentially enhance biol. activity, a series of synthetic and chem. biol. studies were undertaken in order to discover potent antibacterial agents. We describe two ligation methods (disulfide formation and olefin metathesis) for dimerizing vancomycin derivs. and applications of target-accelerated combinatorial synthesis (e.g., combinatorial synthesis in the presence of vancomycin's target Ac2-L-Lys-D-Ala-D-Ala) to generate libraries of vancomycin dimers. Screening of these compd. libraries led to the identification of a no. of highly potent antibiotics effective against vancomycin-susceptible, vancomycin-intermediate resistant and, most significantly, vancomycin-resistant bacteria.

IT 321362-17-8 383183-30-0 383183-31-1  
 383183-32-2 383183-33-3 383183-34-4  
 383183-35-5 383183-36-6 383183-37-7  
 383183-38-8 383183-39-9 383183-40-2  
 383183-41-3 383183-42-4 383183-43-5  
 383183-44-6 383183-45-7 383183-46-8  
 383183-71-9 383183-72-0 383183-73-1  
 383183-74-2 383183-75-3 383183-76-4  
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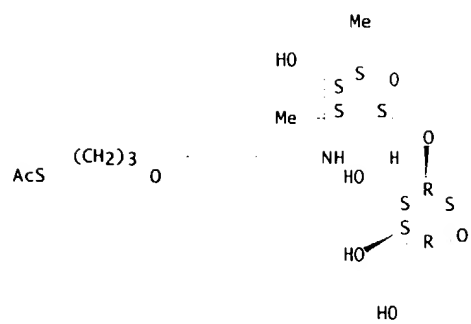
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

RN 321362-17-8 CAPLUS

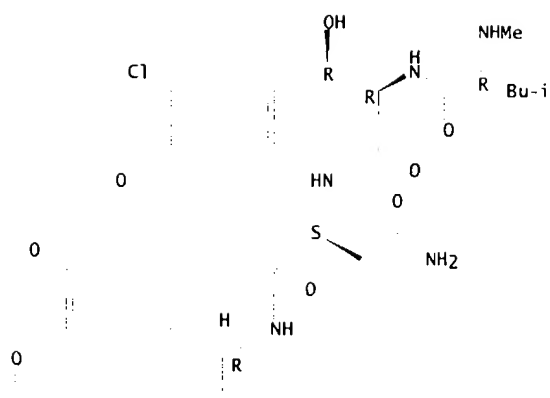
CN Vancomycin, N3''-[3-[3-(acetylthio)propoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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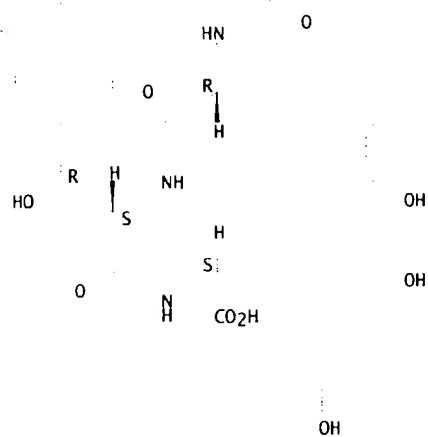


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Cl.



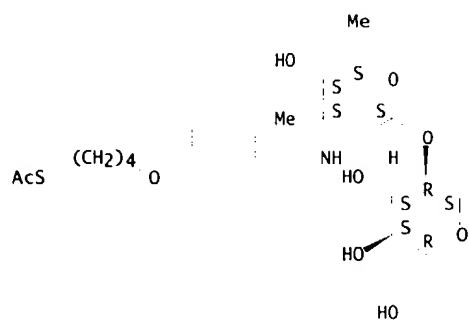
PAGE 2-B



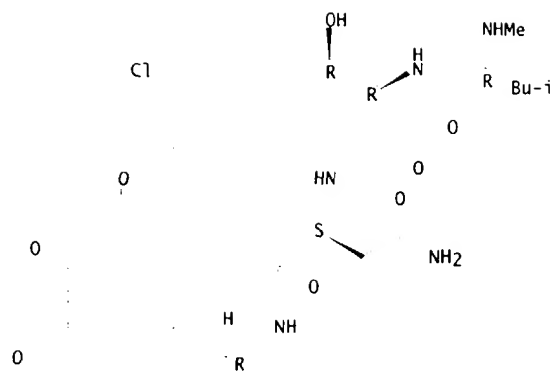
RN 383183-30-0 CAPLUS  
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 INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



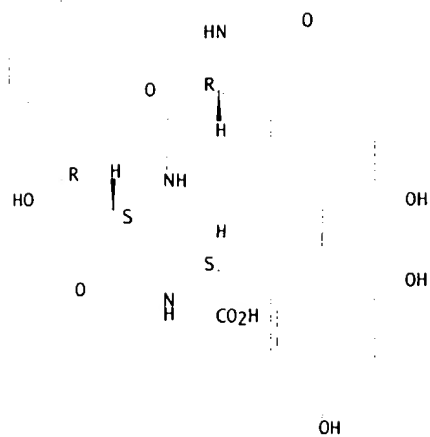
PAGE 1-B



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Cl

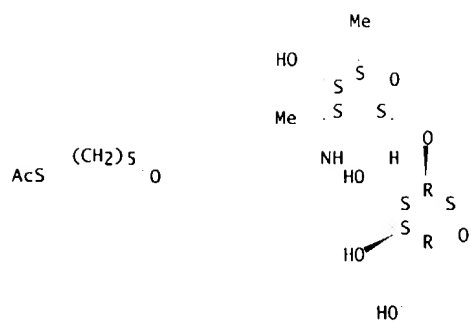
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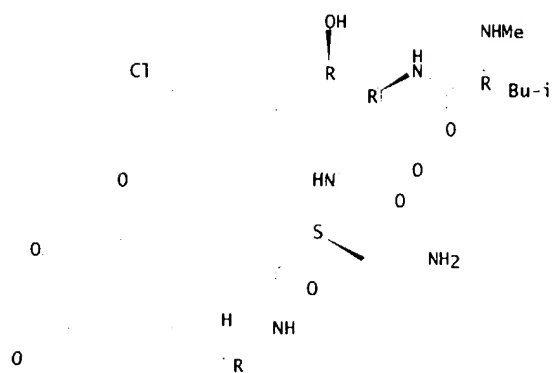
RN 383183-31-1 CAPLUS  
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 INDEX NAME)

Absolute stereochemistry.

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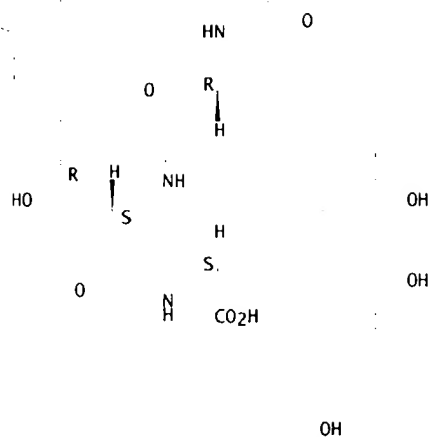
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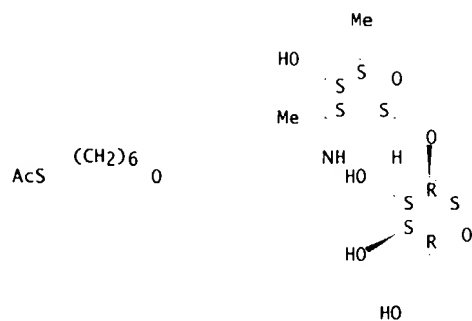
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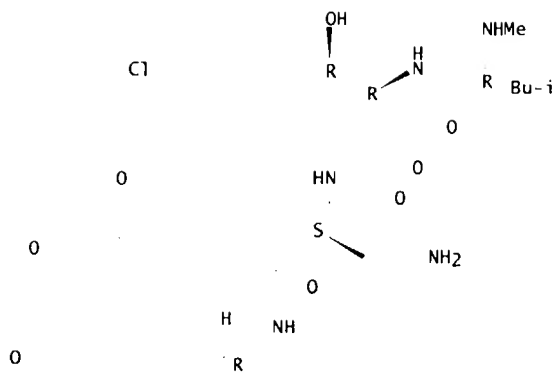
RN 383183-32-2 CAPLUS  
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 INDEX NAME)

Absolute stereochemistry.

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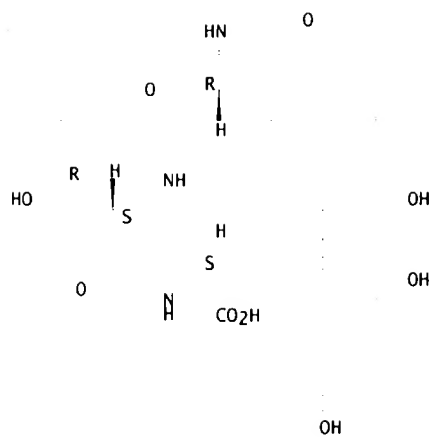
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C1

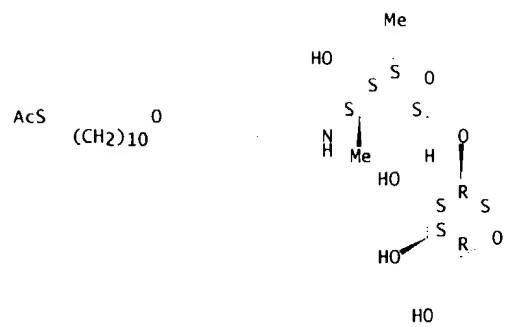
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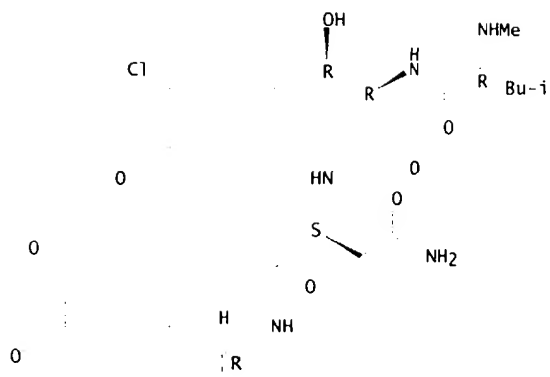
RN 383183-33-3 CAPLUS  
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 INDEX NAME)

Absolute stereochemistry.

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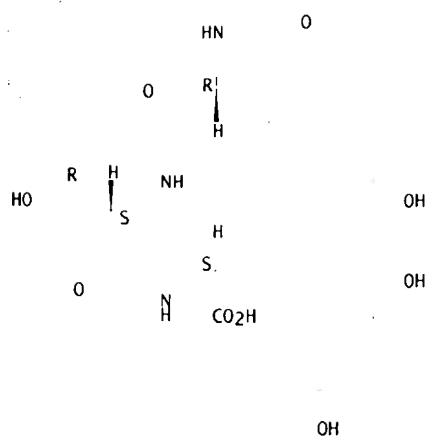
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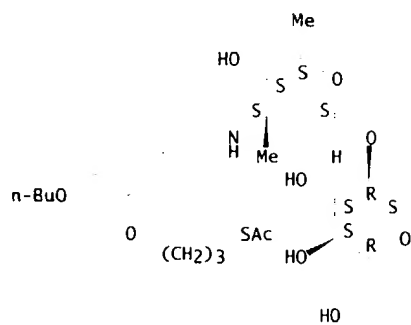
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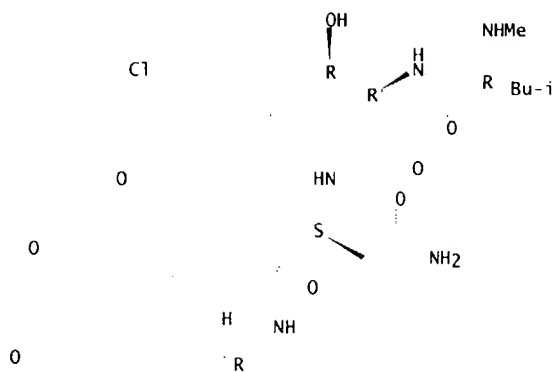
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 (CA INDEX NAME)

Absolute stereochemistry.

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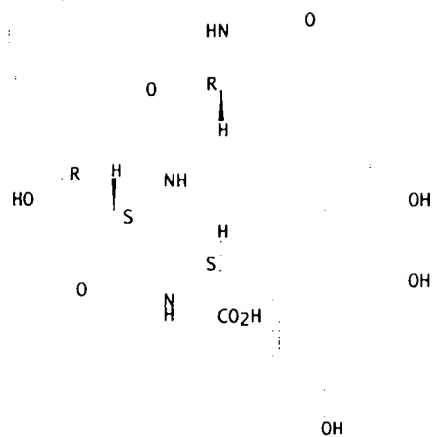
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C1

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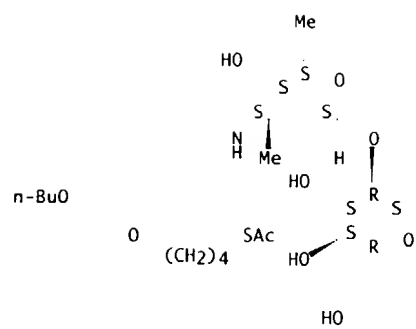


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 (CA INDEX NAME)

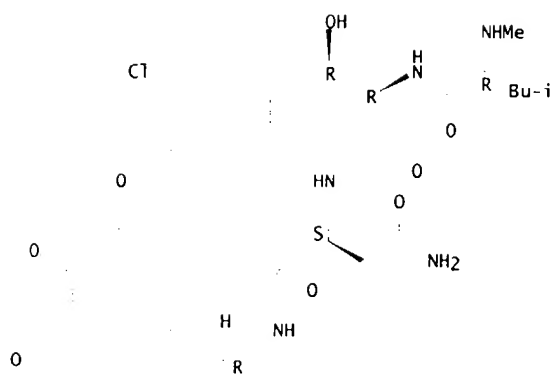
Absolute stereochemistry.



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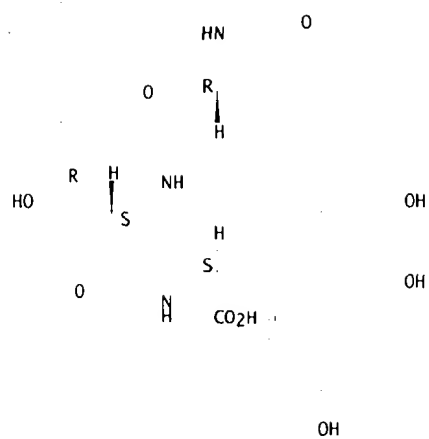
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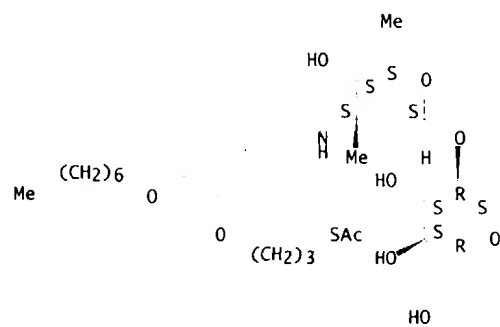
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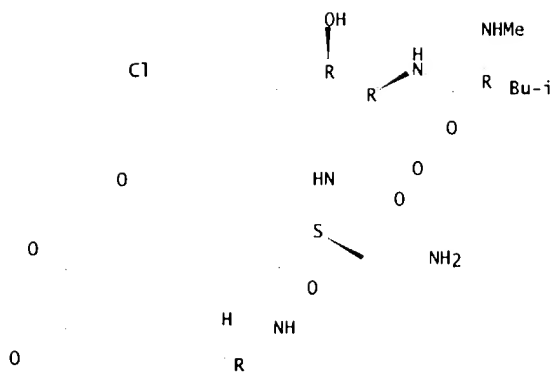
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 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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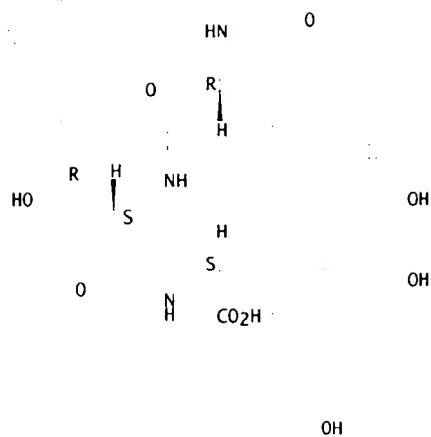
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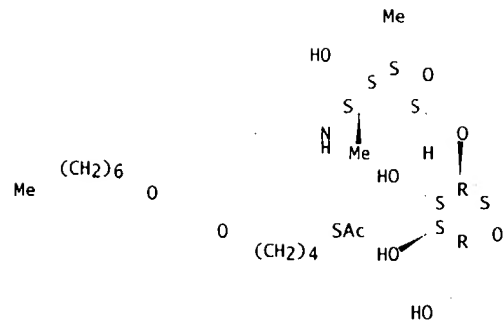
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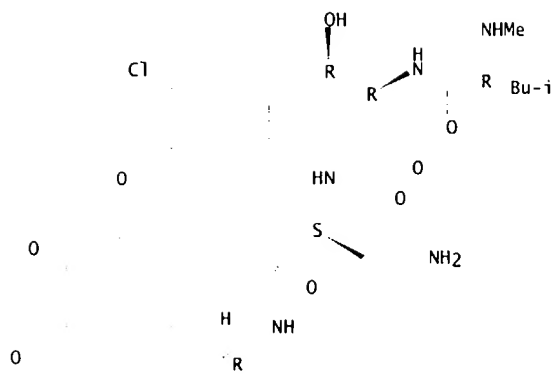
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 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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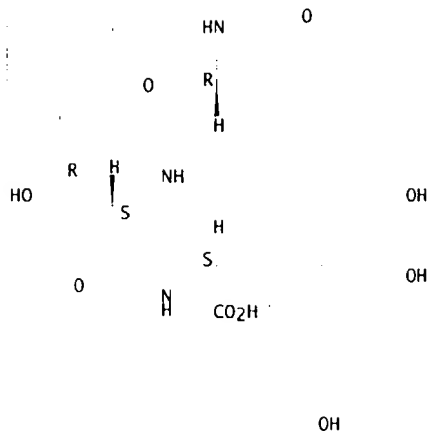


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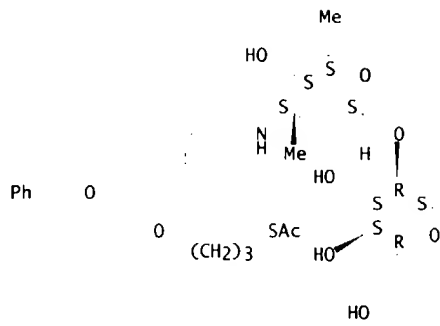
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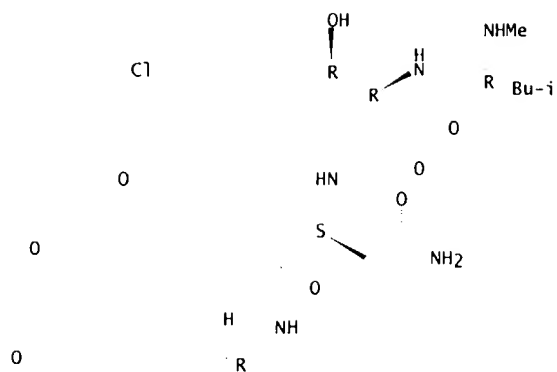


RN 383183-38-8 CAPLUS  
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Absolute stereochemistry.



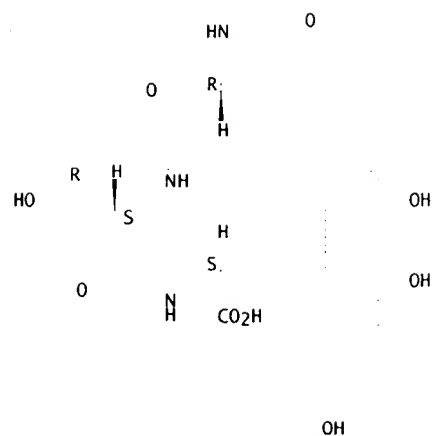
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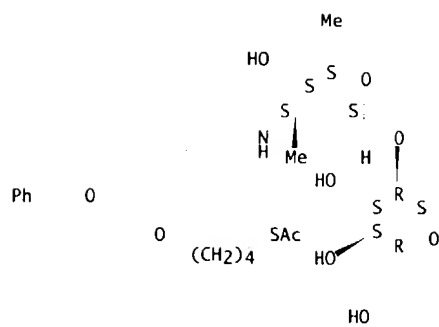
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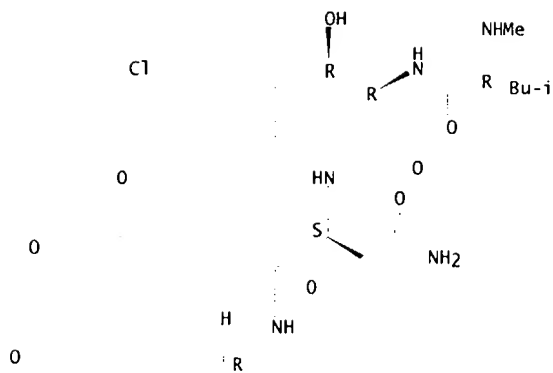
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Absolute stereochemistry.

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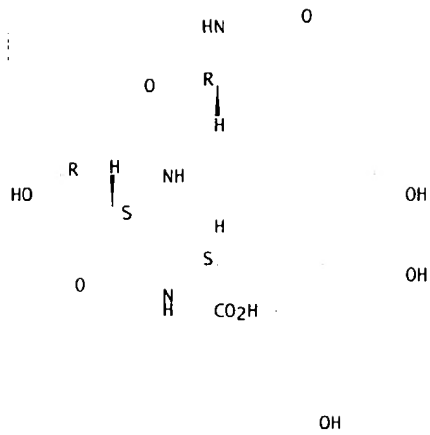
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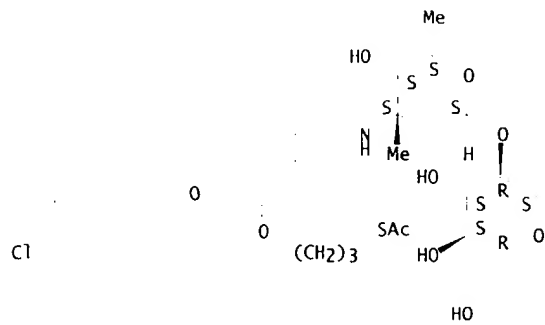
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RN 383183-40-2 CAPLUS  
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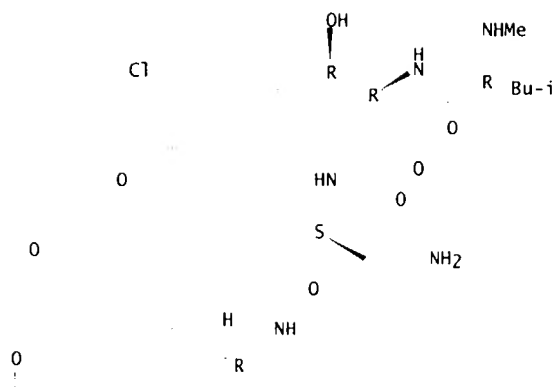
Absolute stereochemistry.

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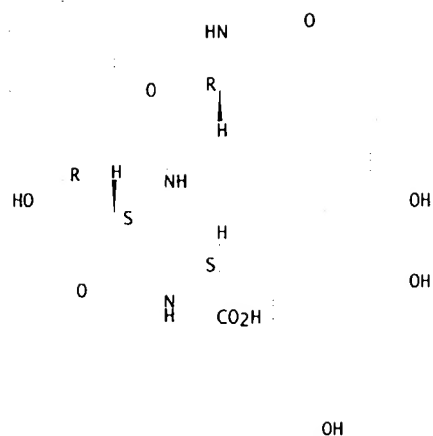
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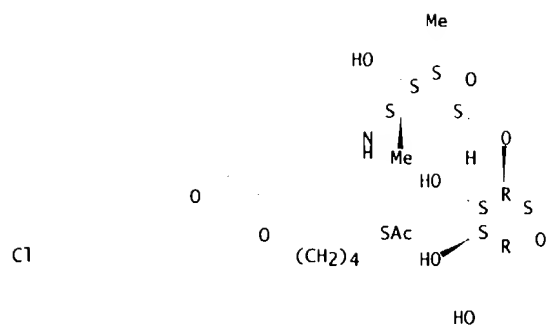
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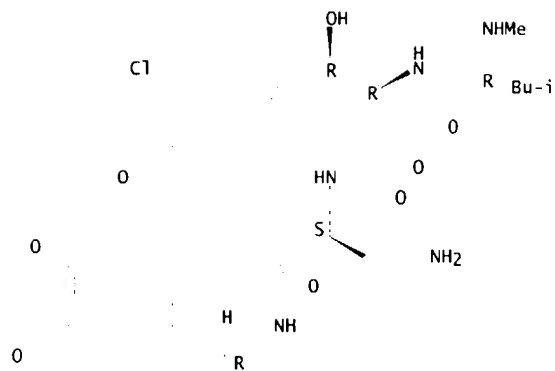
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Absolute stereochemistry.

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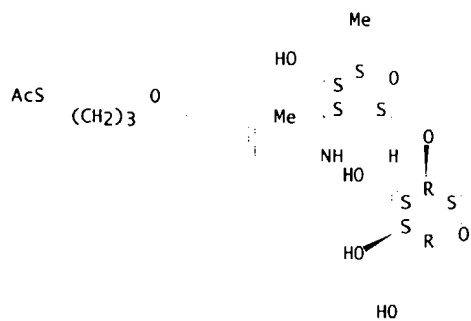


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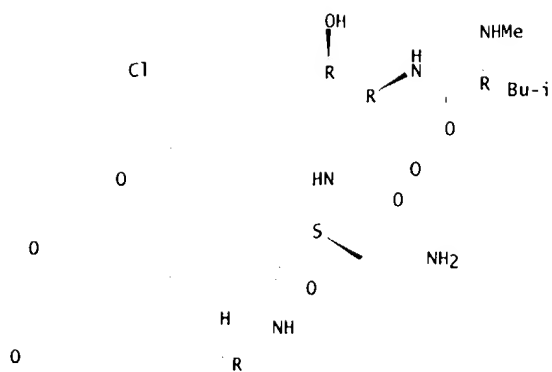
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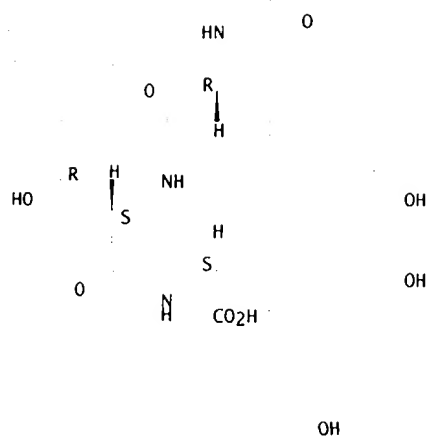
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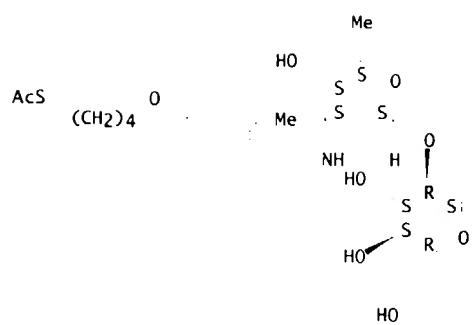
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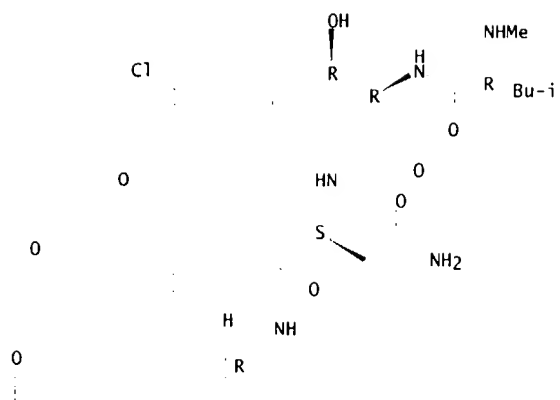
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 INDEX NAME)

Absolute stereochemistry.

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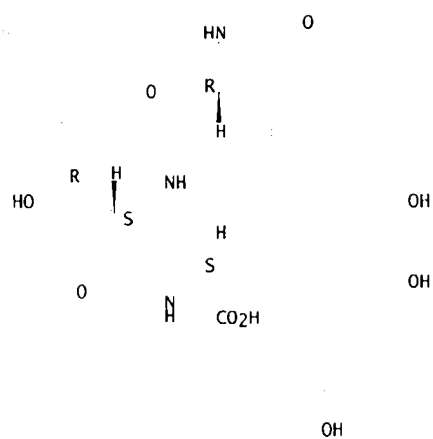
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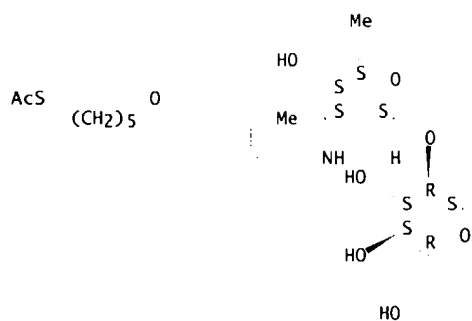
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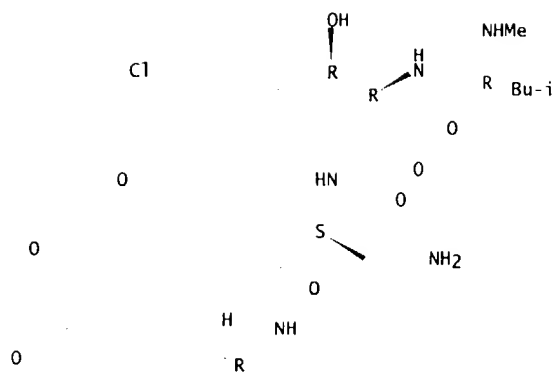
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 INDEX NAME)

Absolute stereochemistry.

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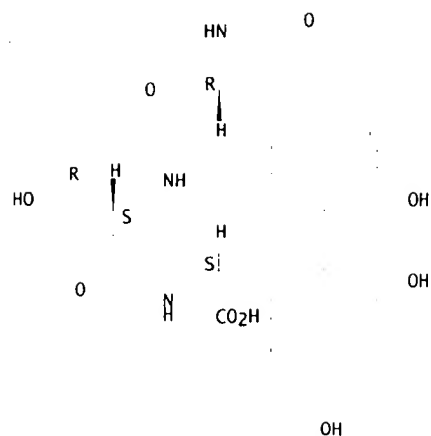
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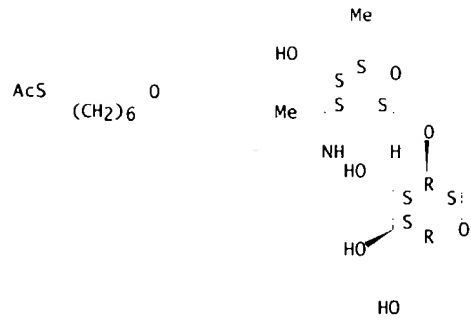
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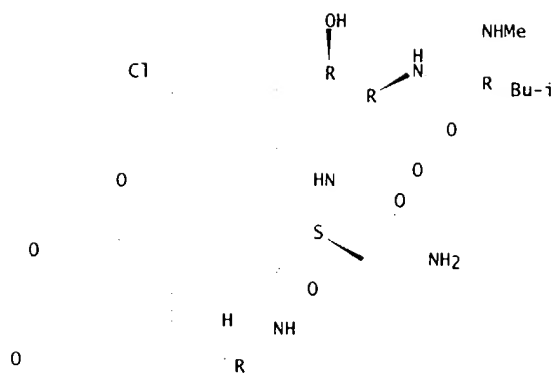
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 CN Vancomycin, N3'''-[[4-[[6-(acetylthio)hexyl]oxy]phenyl]methyl]- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

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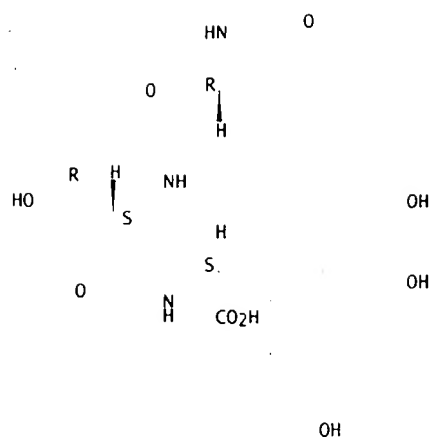


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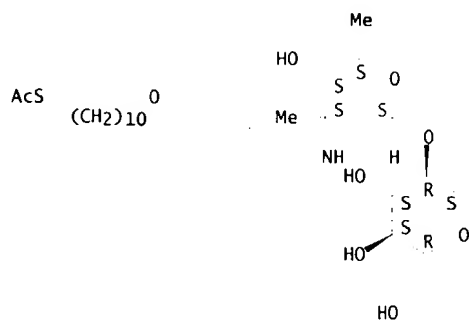
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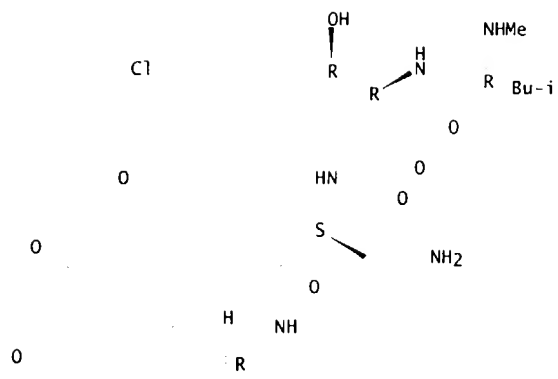
RN 383183-46-8 CAPLUS  
 CN Vancomycin, N3'''-[[4-[[10-(acetylthio)decyl]oxy]phenyl]methyl]- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

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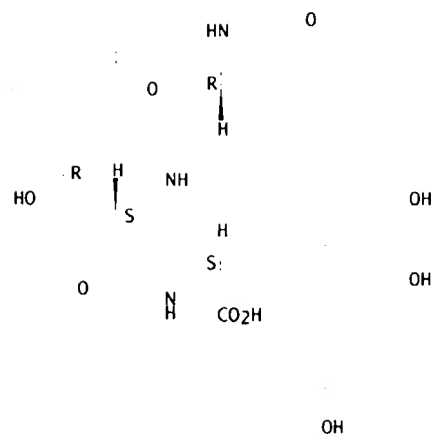
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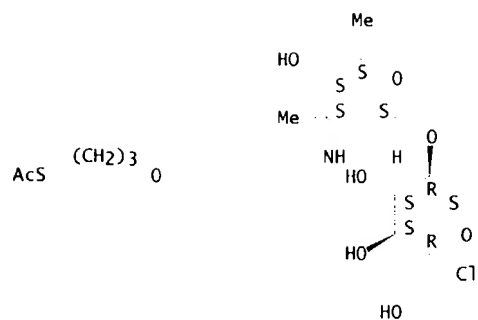
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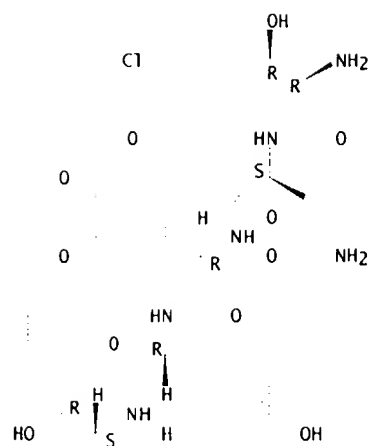
RN 383183-71-9 CAPLUS  
 CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-  
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 (methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

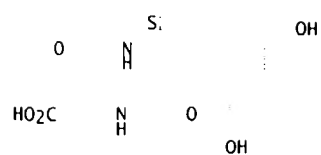
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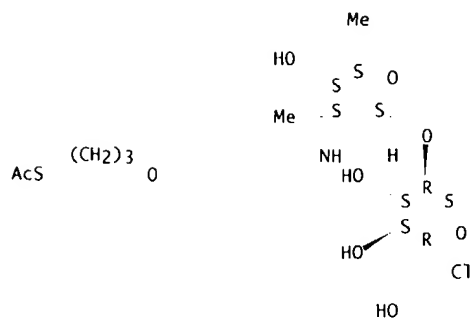
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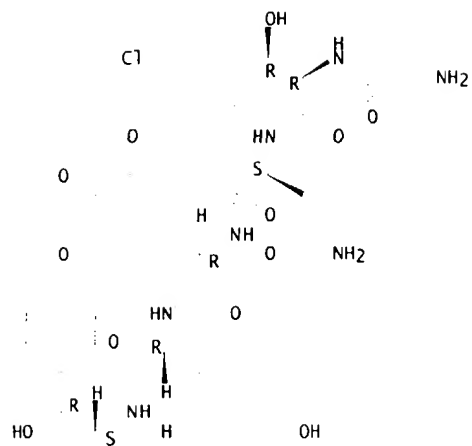
RN 383183-72-0 CAPLUS  
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Absolute stereochemistry.

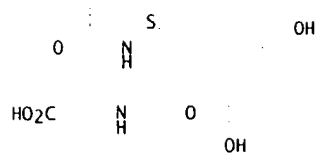
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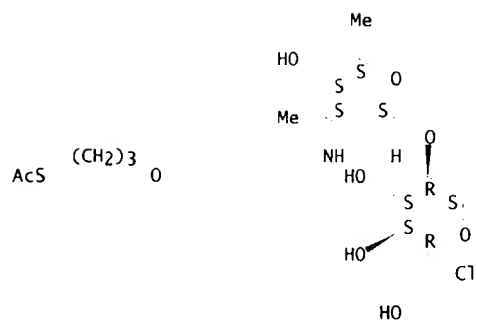


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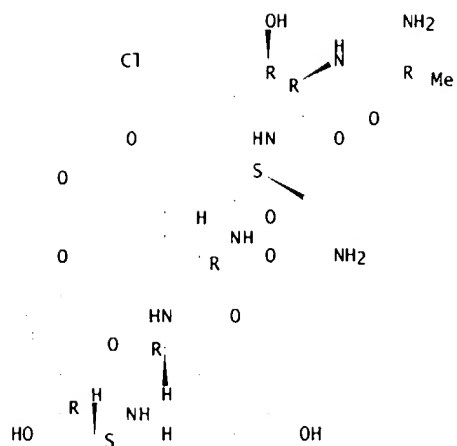
CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2R)-2-amino-1-oxopropyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

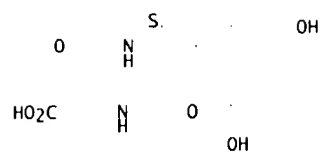
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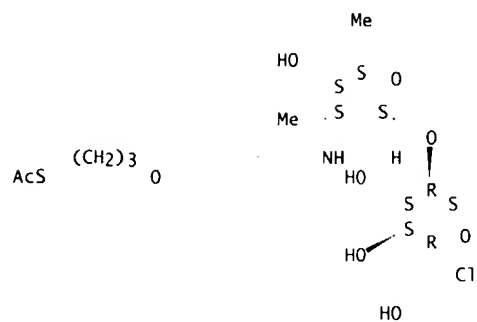


RN 383183-74-2 CAPLUS

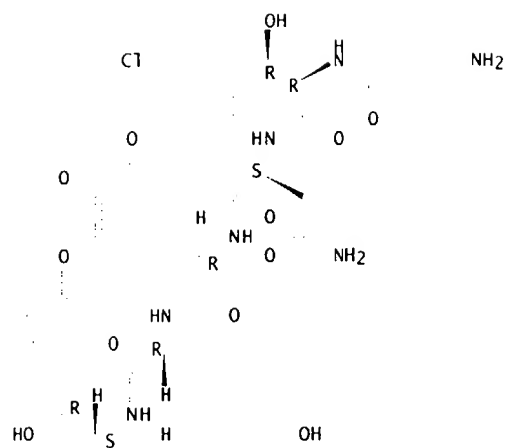
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(3-amino-1-oxopropyl)-28-[[[carboxymethyl]amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

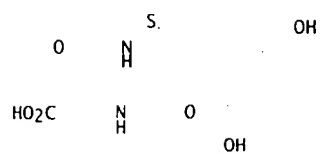
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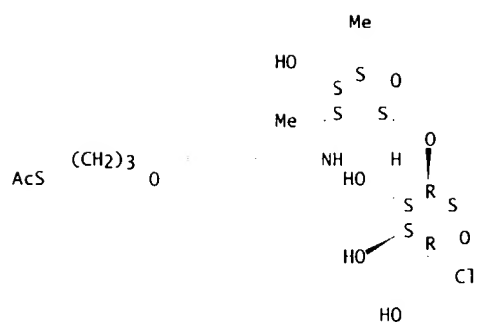
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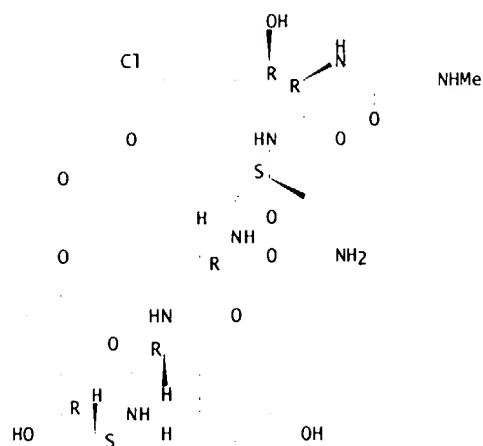
RN 383183-75-3 CAPLUS  
 CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-  
 [[[carboxymethyl]amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-  
 (methylamino)-1-oxopentyl]-49-[(methylamino)acetyl]- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.

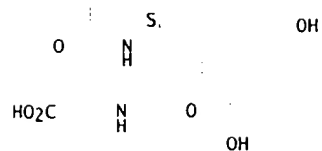
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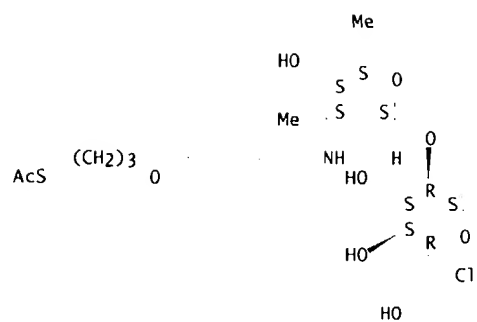


RN 383183-76-4 CAPLUS

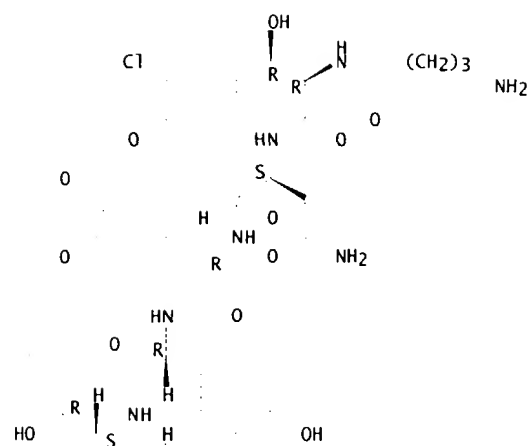
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Absolute stereochemistry.

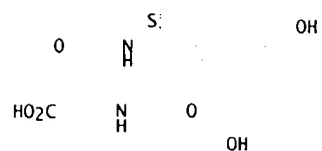
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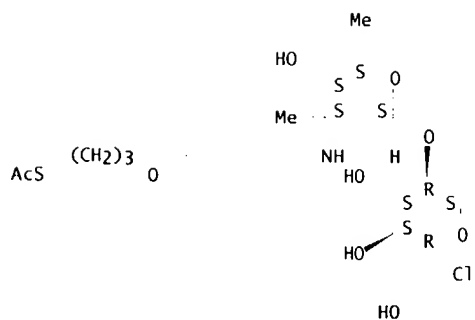


RN 383183-77-5 CAPLUS  
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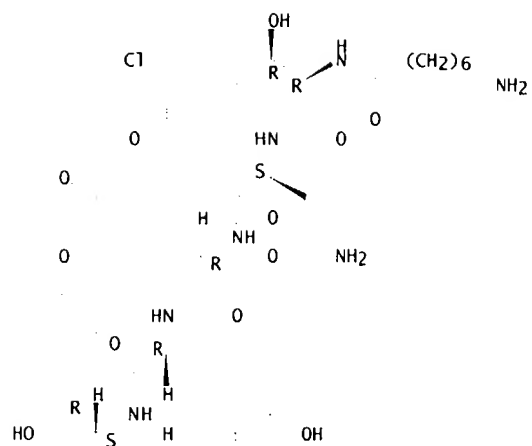
Absolute stereochemistry.



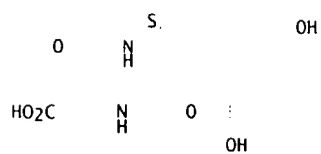
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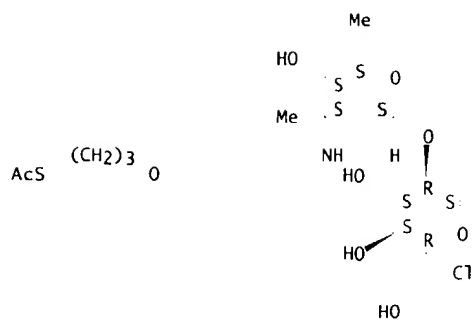
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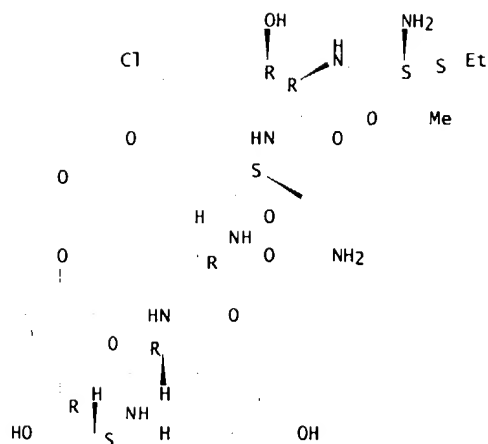
RN 383183-78-6 CAPLUS  
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Absolute stereochemistry.

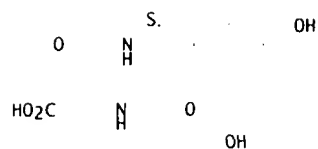
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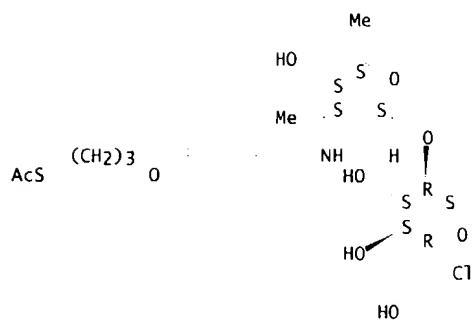
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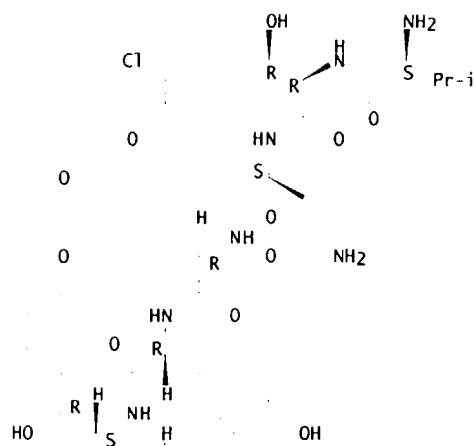
RN 383183-79-7 CAPLUS  
 CN Vancomycin, N3' '-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-methyl-1-oxobutyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

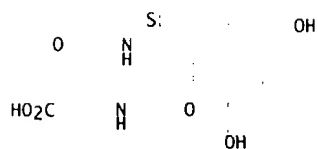
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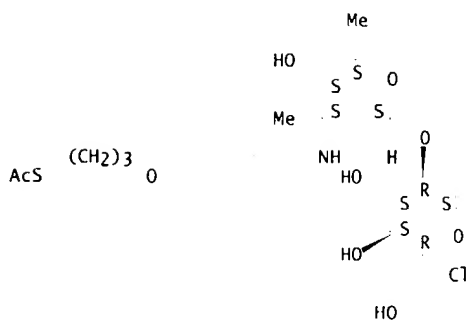


RN 383183-80-0 CAPLUS

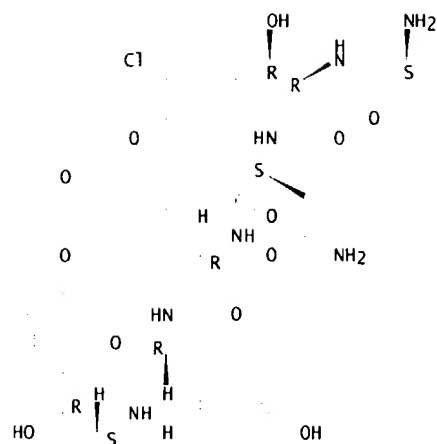
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Absolute stereochemistry.

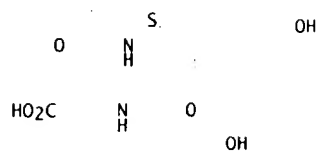
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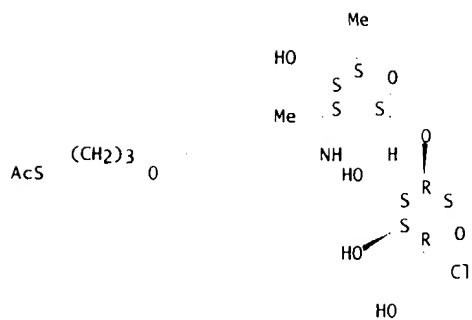
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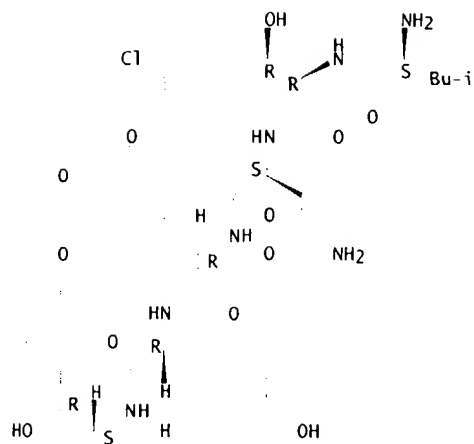
RN 383183-81-1 CAPLUS  
 CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-  
 [[[(carboxymethyl)amino]carbonyl]-28-decarboxy-56-demethyl-, (51S)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.

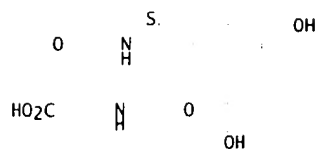
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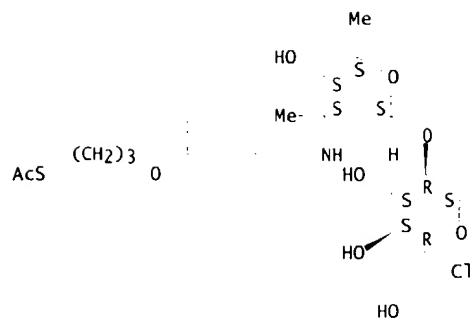
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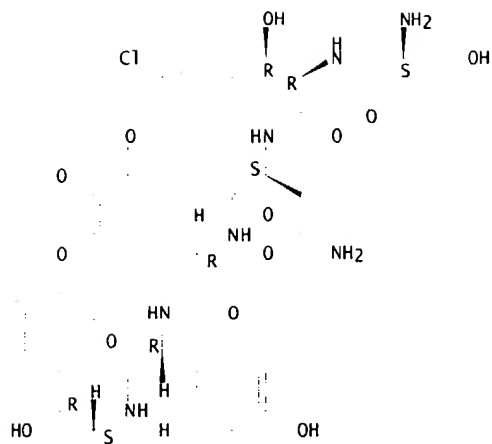
RN 383183-82-2 CAPLUS  
 CN Vancomycin, N3''-[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-hydroxy-1-oxopropyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

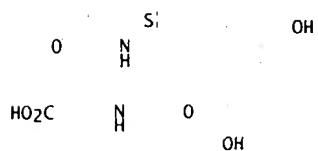
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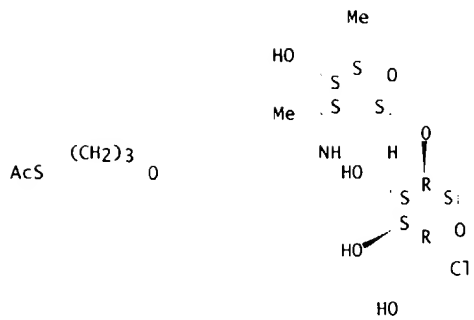
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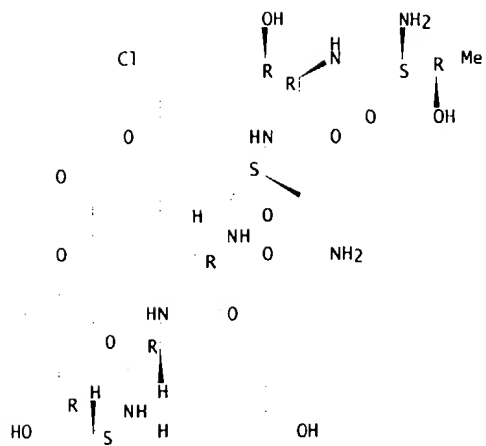
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Absolute stereochemistry.

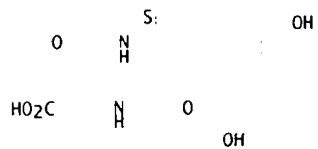
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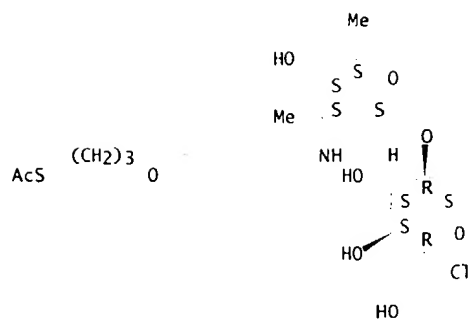
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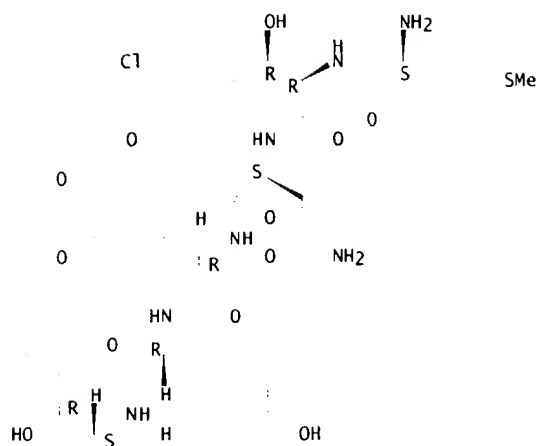
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Absolute stereochemistry.

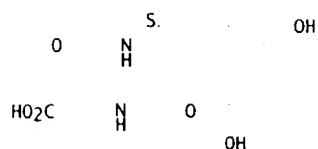
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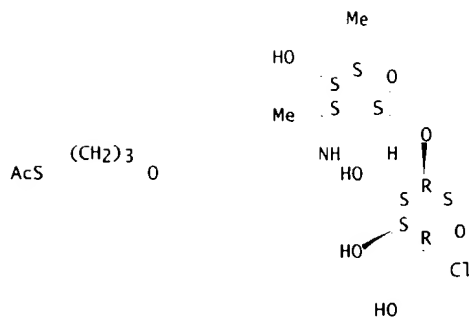


RN 383184-99-4 CAPLUS  
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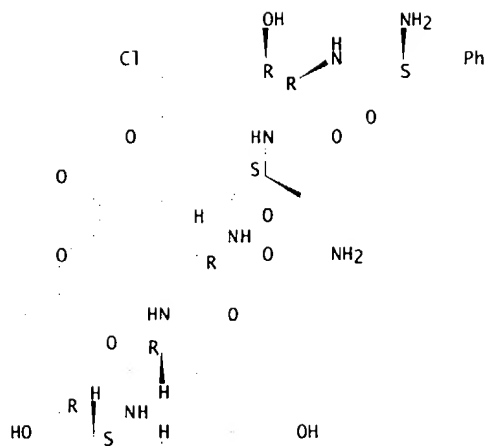
Absolute stereochemistry.



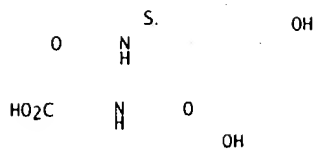
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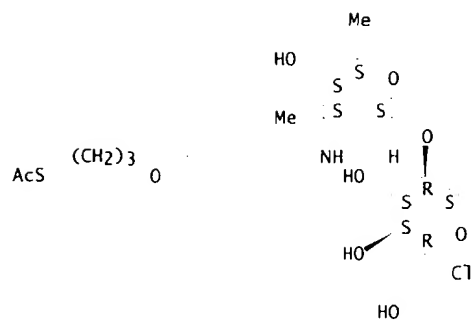
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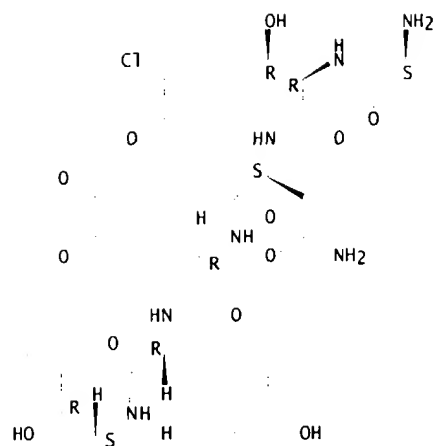
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CN Vancomycin, N3''-[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-(4-hydroxyphenyl)-1-oxopropyl]-26-[[[carboxymethyl]amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

**Absolute stereochemistry.**

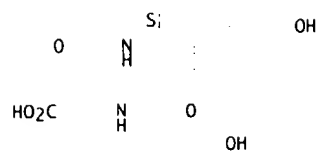
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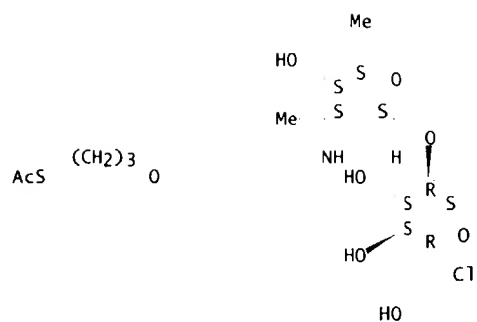
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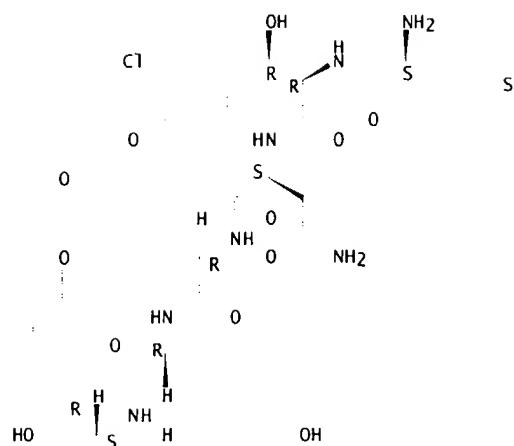
RN 383185-06-6 CAPLUS  
 CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-1-oxo-3-(2-thienyl)propyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

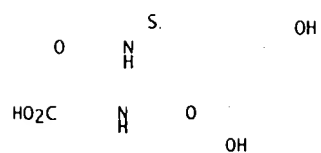
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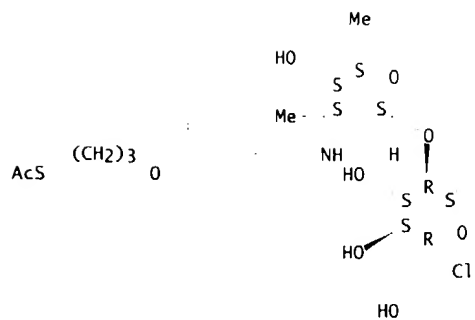
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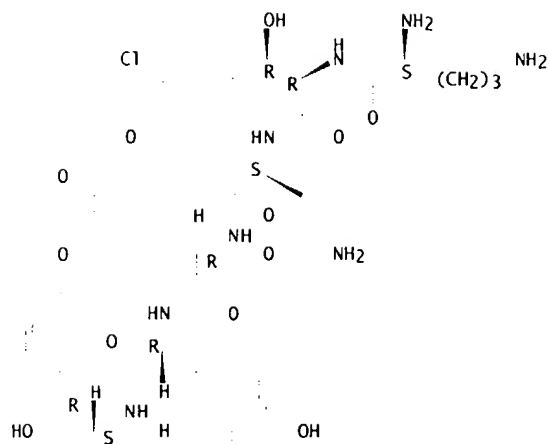
RN 383185-07-7 CAPLUS  
 CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-amino-26-  
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 INDEX NAME)

Absolute stereochemistry.

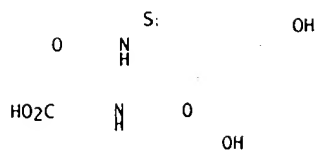
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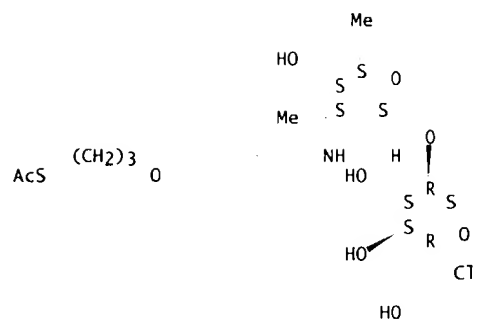
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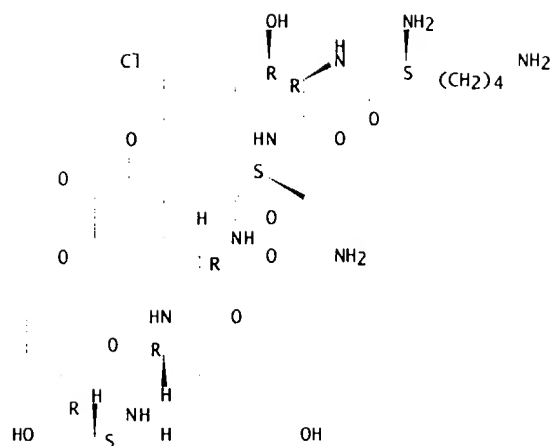
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 (methylamino)-1-oxopentyl]-49-[(2S)-2,6-diamino-1-oxohexyl]- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

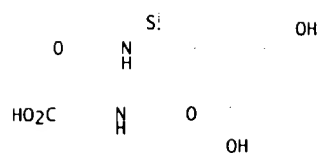
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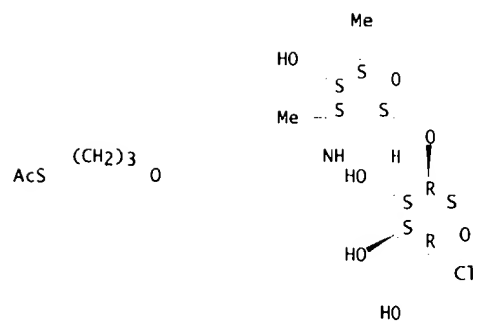
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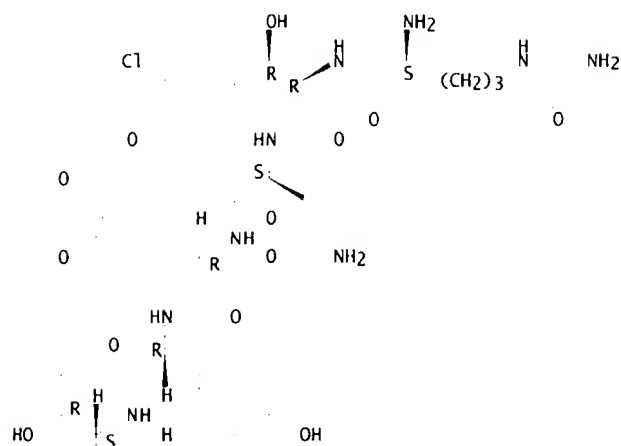
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Absolute stereochemistry.

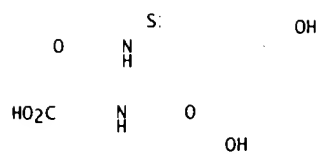
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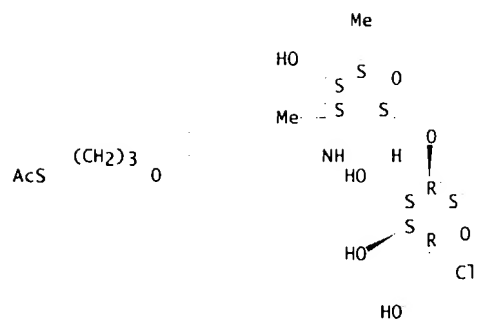
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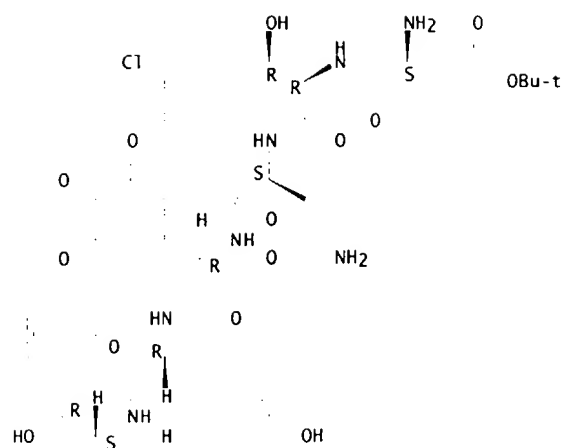
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Absolute stereochemistry.

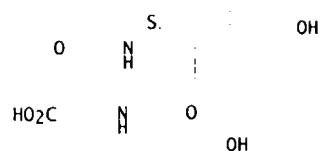
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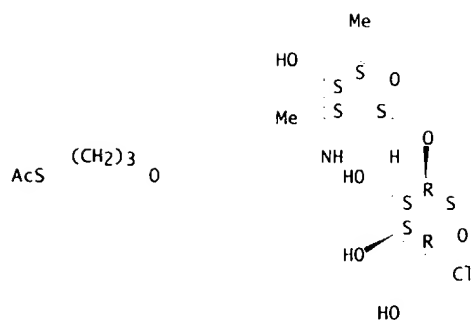


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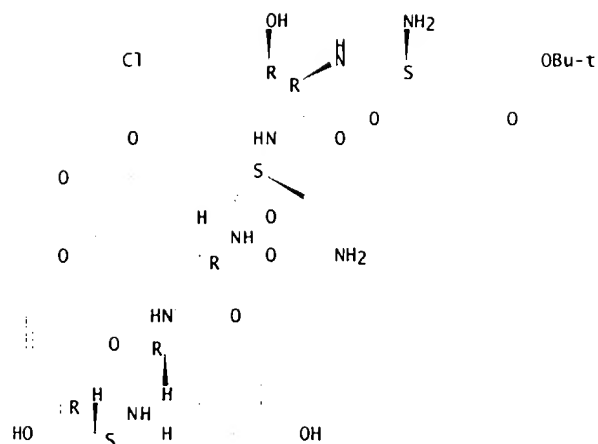
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Absolute stereochemistry.

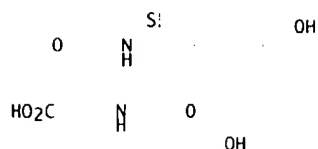
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REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:689110 CAPLUS

DOCUMENT NUMBER: 136:70059

TITLE: Solid- and solution-phase synthesis of vancomycin and vancomycin analogues with activity against vancomycin-resistant bacteria

AUTHOR(S): Nicolaou, K. C.; Cho, Suk Young; Hughes, Robert; Winssinger, Nicolas; Smethurst, Christian; Labischinski, Harald; Endermann, Rainer

CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Chemistry--A European Journal (2001), 7(17), 3798-3823 CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English



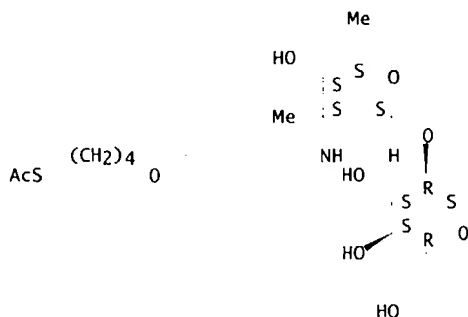
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383183-33-3 383183-34-4 383183-35-5  
383183-36-6 383183-37-7 383183-38-8  
383183-39-9 383183-40-2 383183-41-3  
383183-45-7 383183-46-8 383183-76-4

RL: PAC (Pharmacological activity); BIOL (Biological study)  
(synthesis of vancomycin and vancomycin analogs with activity against  
vancomycin-resistant bacteria)

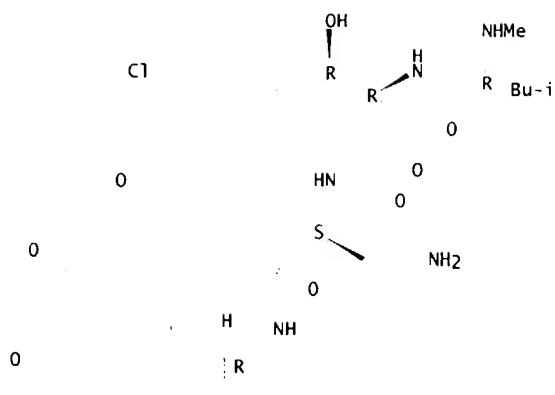
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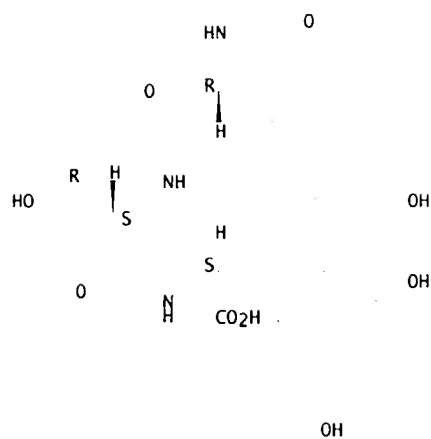
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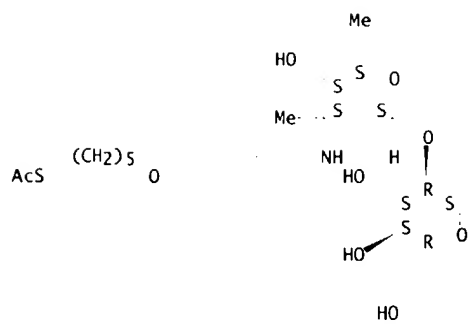
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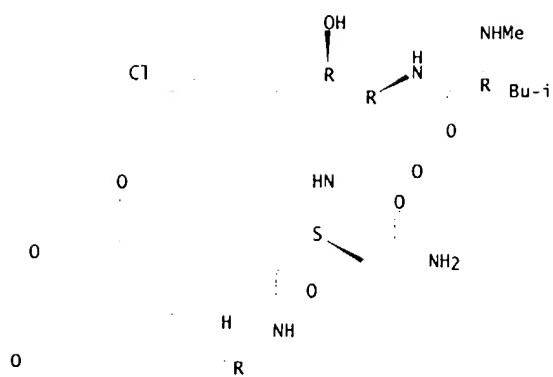
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 INDEX NAME)

Absolute stereochemistry.

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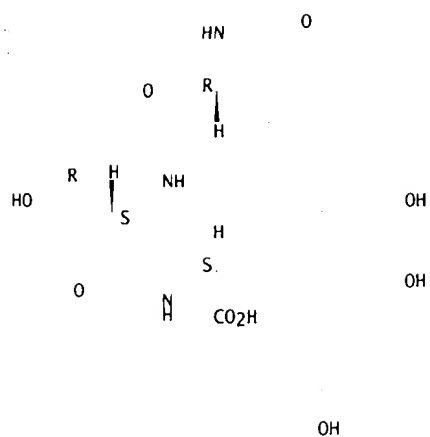
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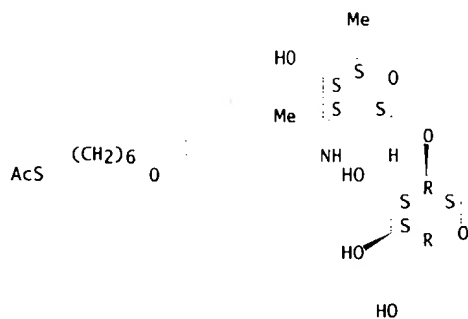
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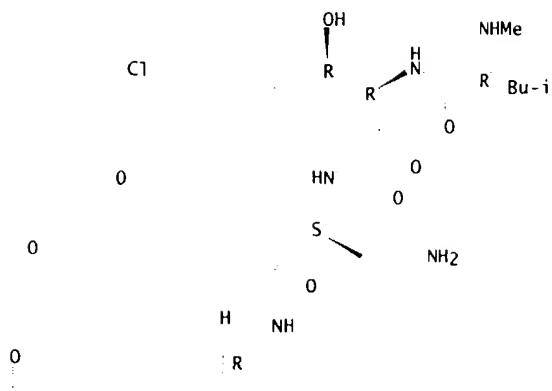
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 INDEX NAME)

Absolute stereochemistry.

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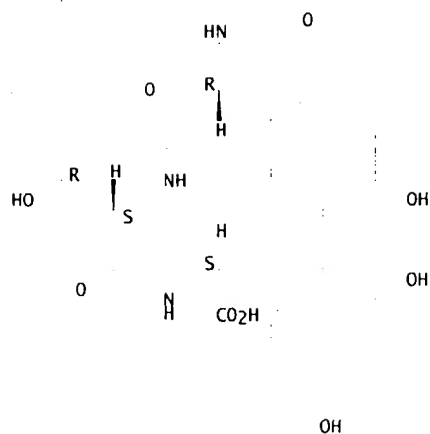
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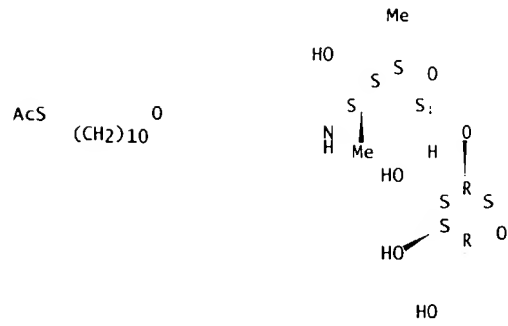
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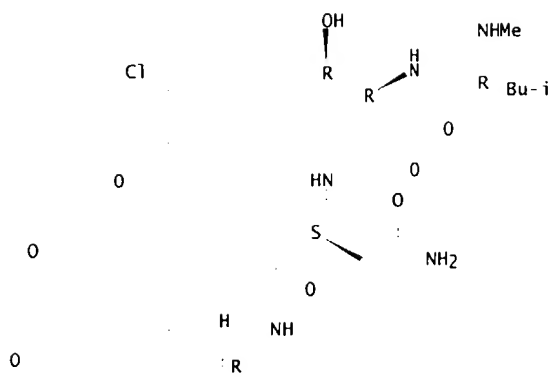
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 INDEX NAME)

Absolute stereochemistry.

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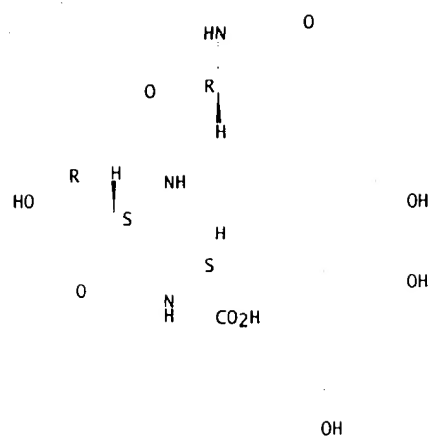
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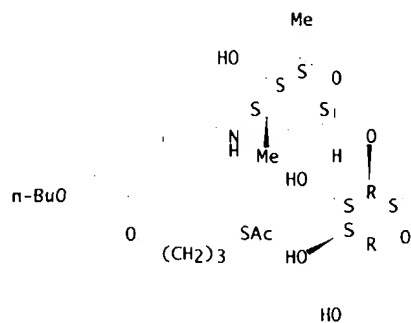
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 (CA INDEX NAME)

Absolute stereochemistry.

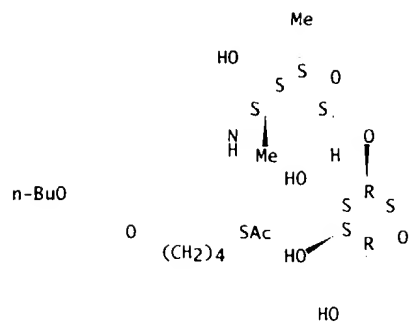
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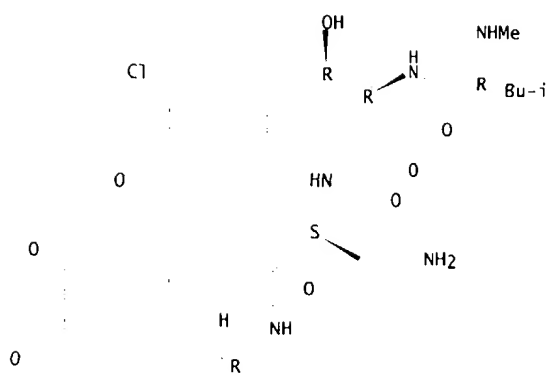




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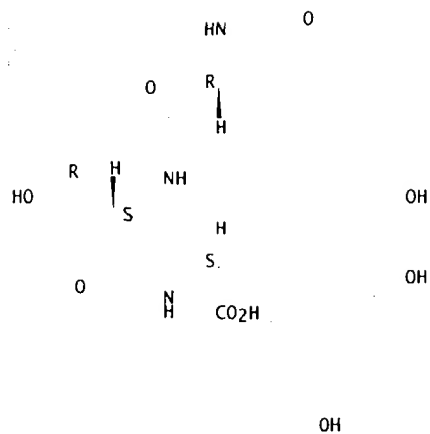
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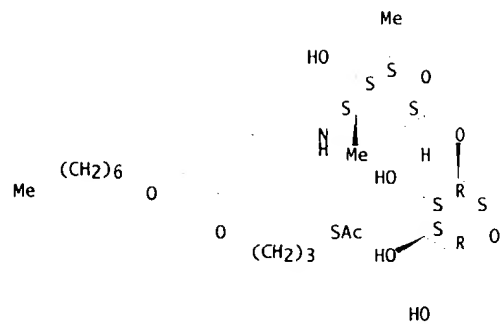
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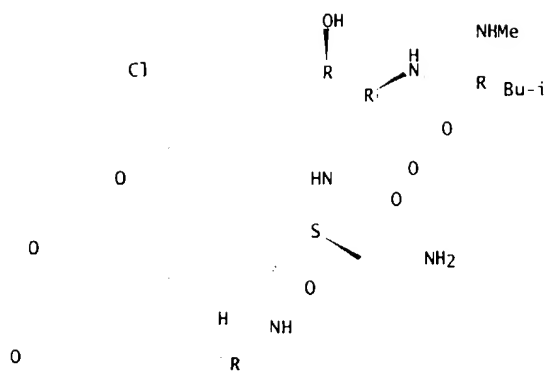
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 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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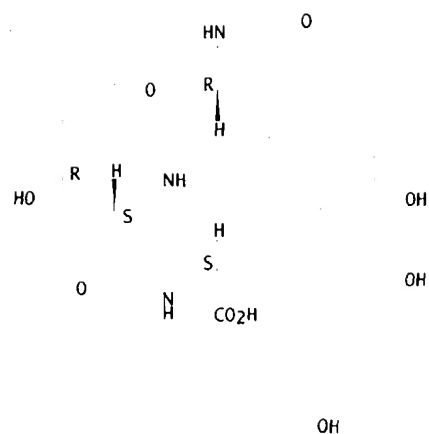
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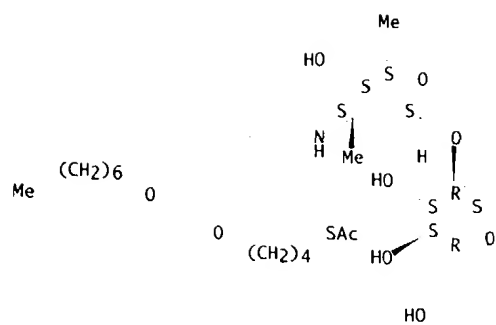


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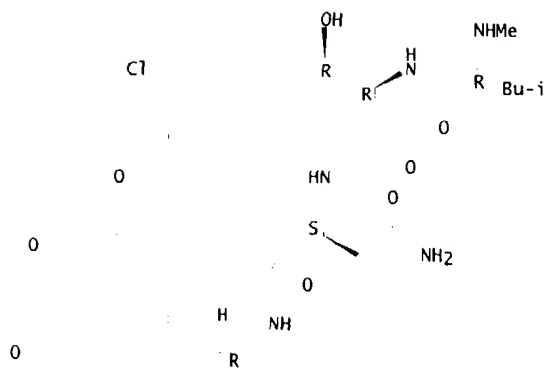
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(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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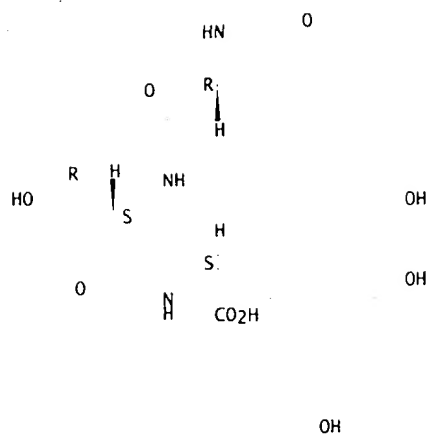
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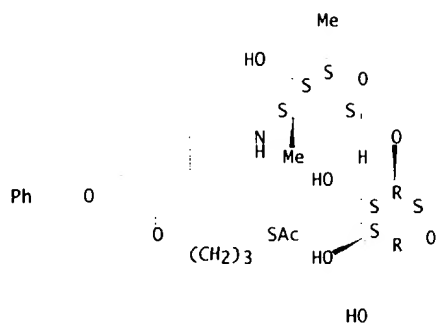
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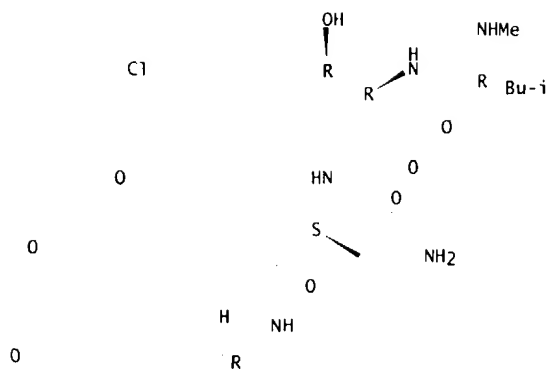
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Absolute stereochemistry.

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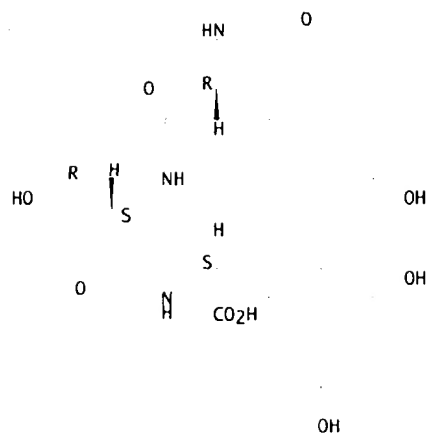
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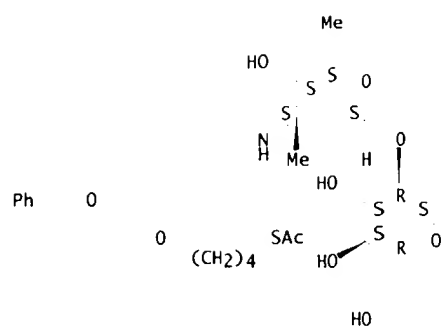
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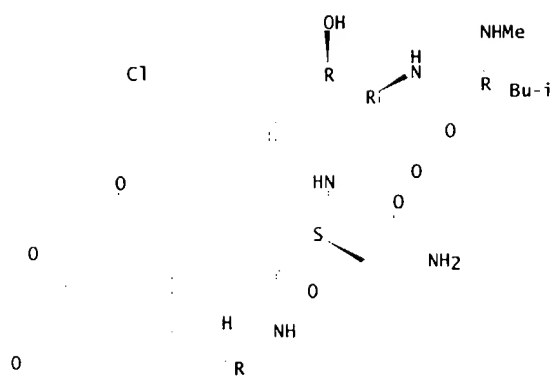
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Absolute stereochemistry.

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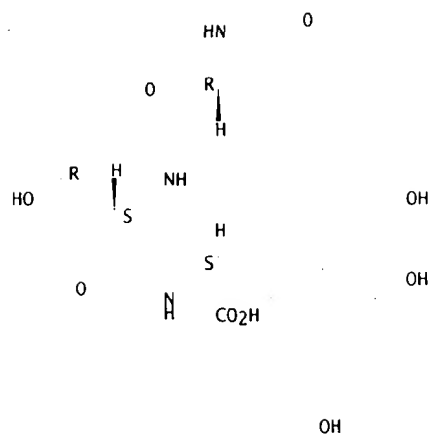
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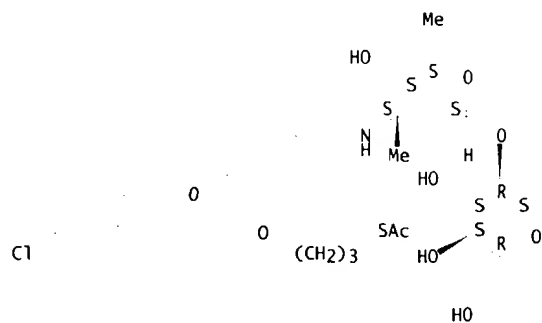
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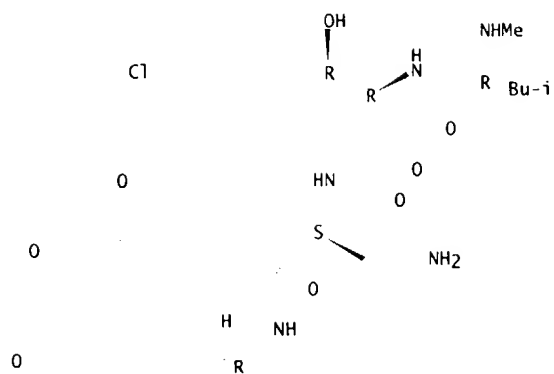
Absolute stereochemistry.

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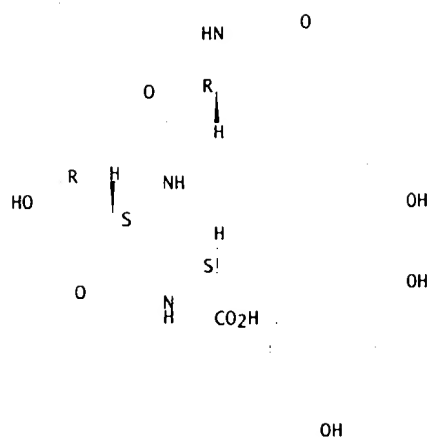
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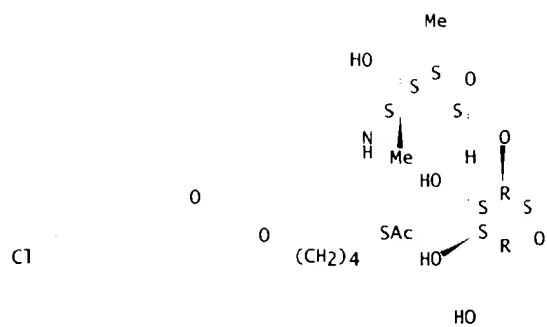
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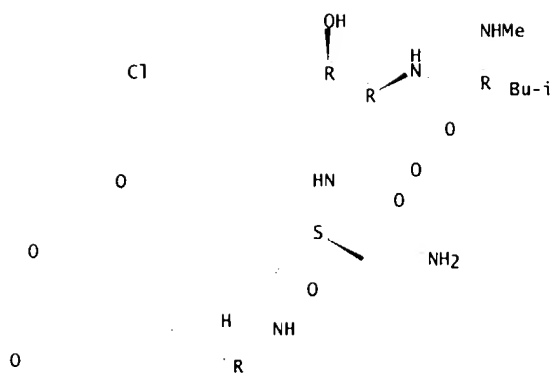
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Absolute stereochemistry.

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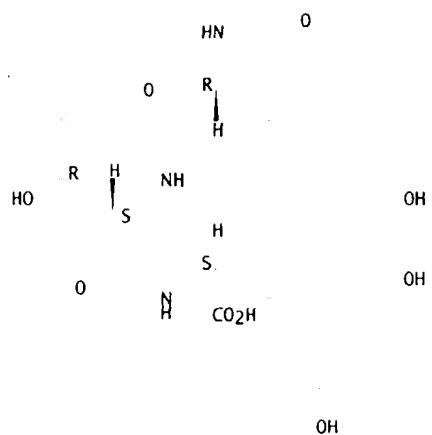
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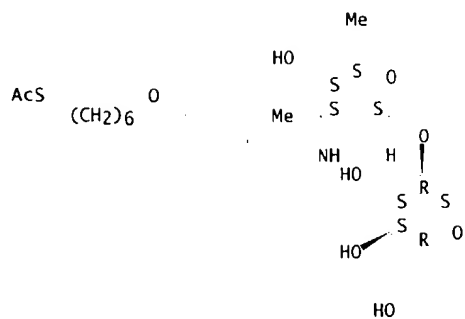
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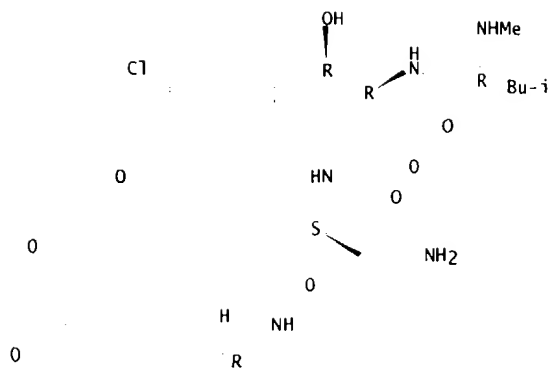
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 INDEX NAME)

Absolute stereochemistry.

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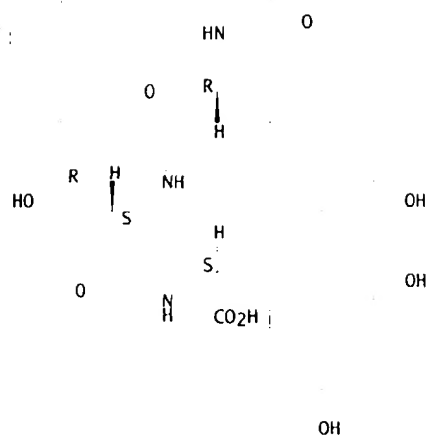
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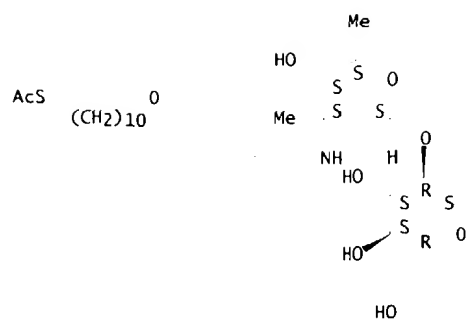
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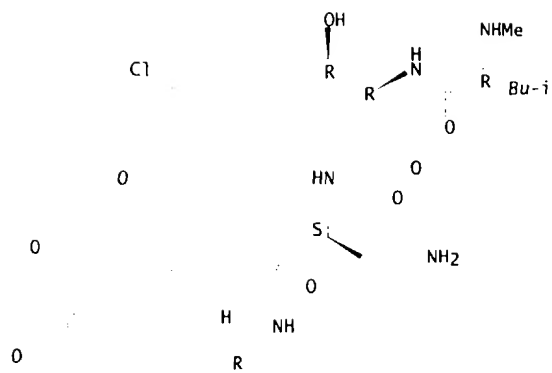
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 INDEX NAME)

Absolute stereochemistry.

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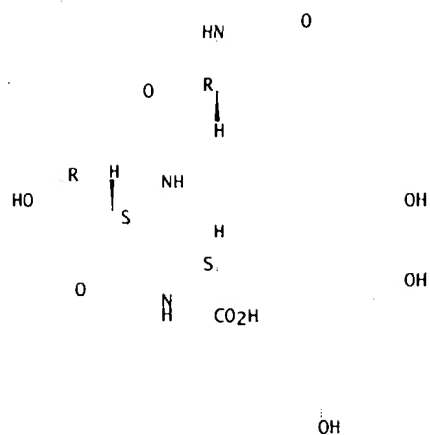
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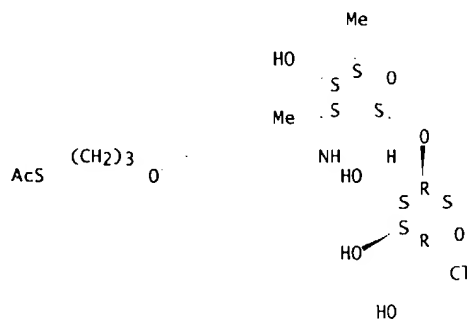


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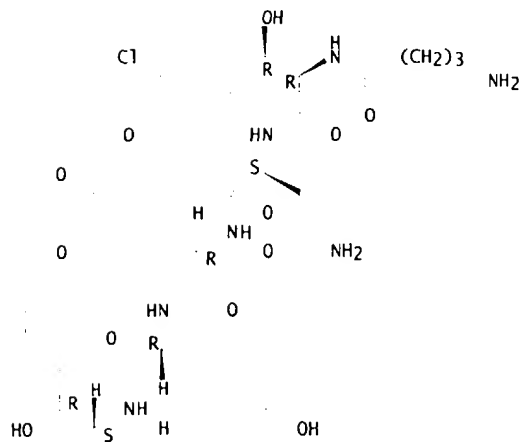
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Absolute stereochemistry.

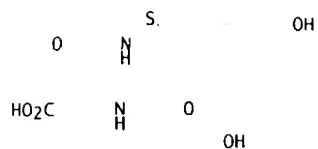
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IT 321362-17-8P

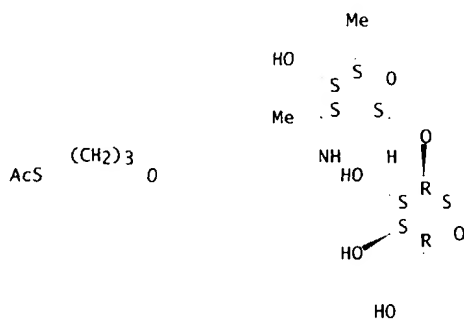
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
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RN 321362-17-8 CAPLUS

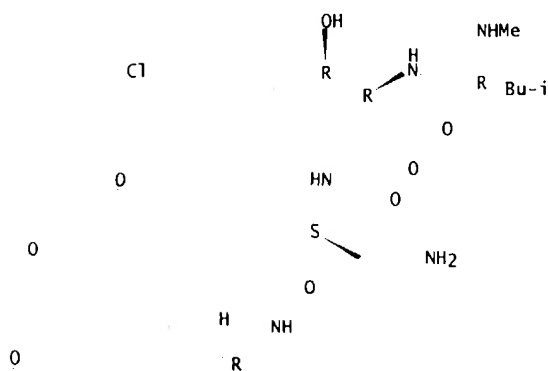
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Absolute stereochemistry.

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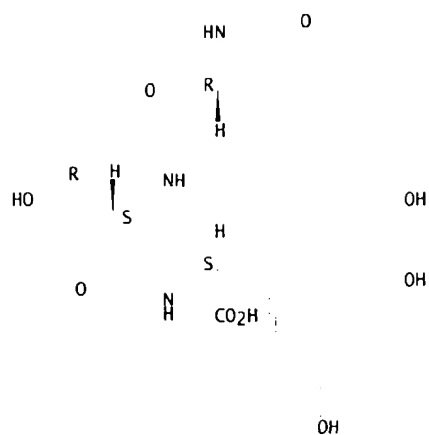
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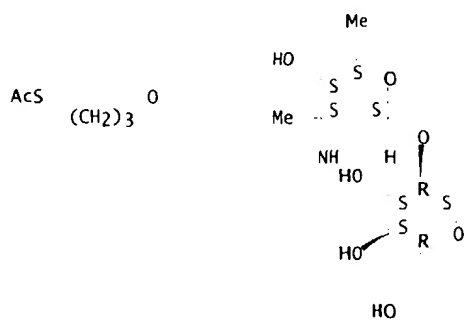
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
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 INDEX NAME)

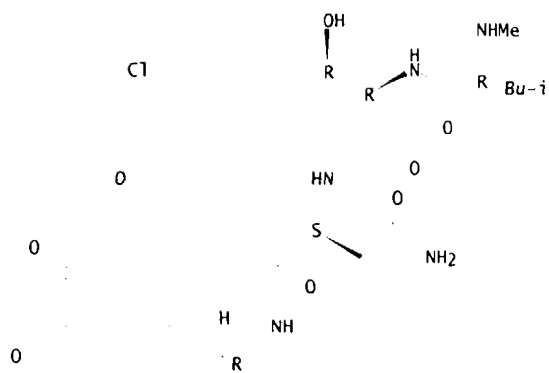
Absolute stereochemistry.

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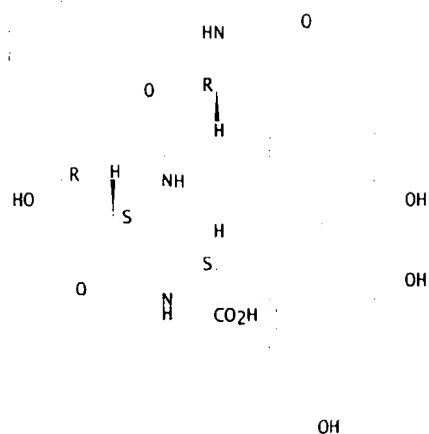
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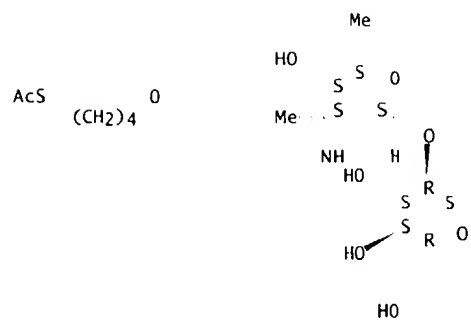
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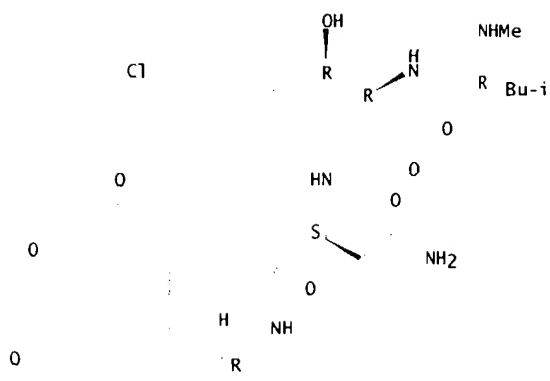
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 INDEX NAME)

Absolute stereochemistry.

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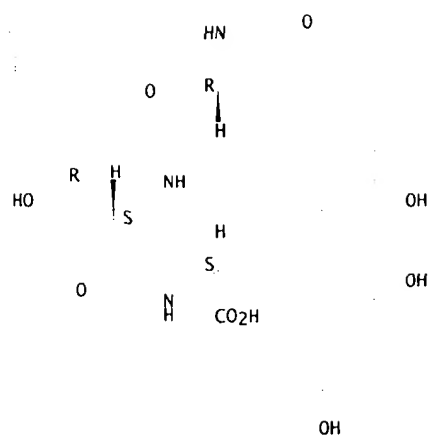


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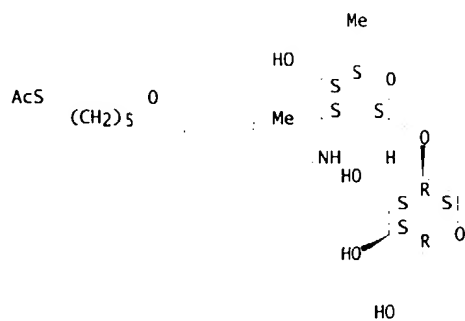
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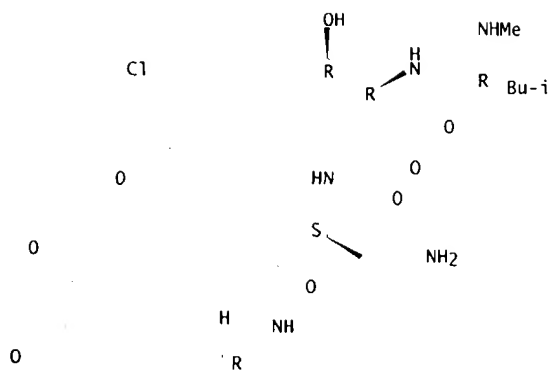


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 INDEX NAME)

Absolute stereochemistry.



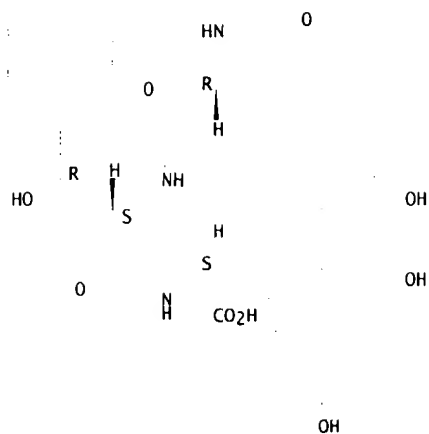
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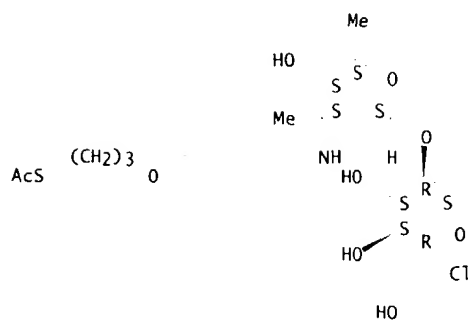
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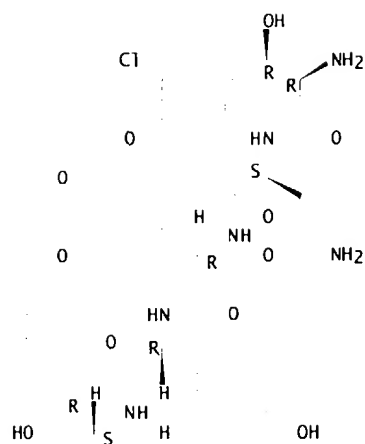
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Absolute stereochemistry.

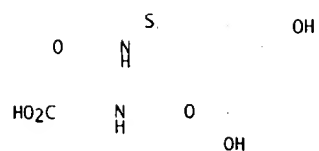
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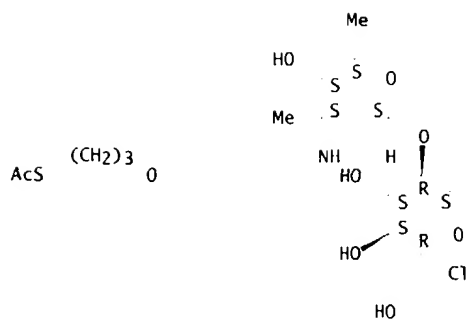


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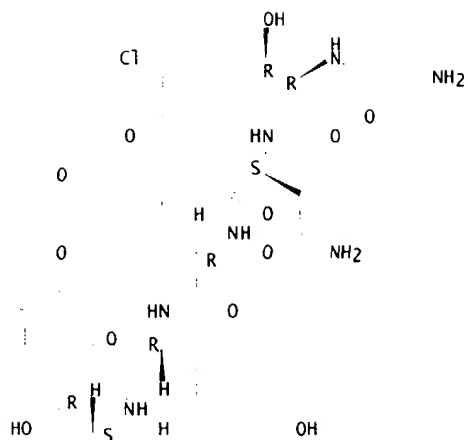
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Absolute stereochemistry.

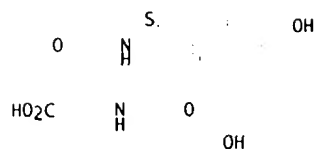
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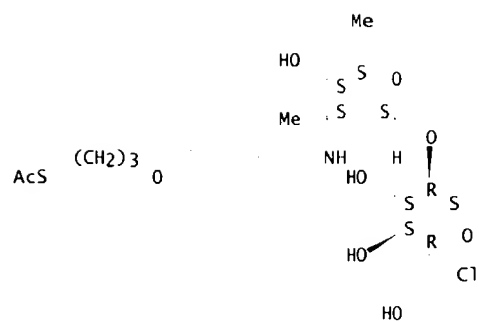
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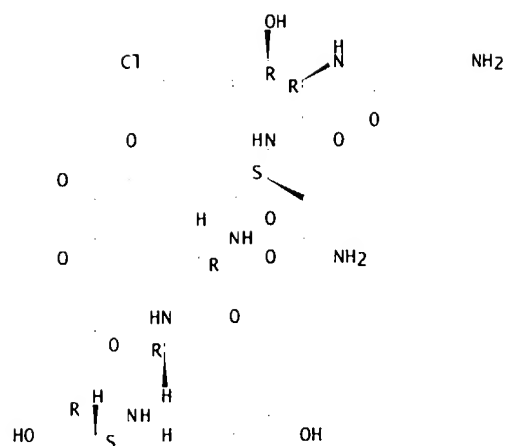
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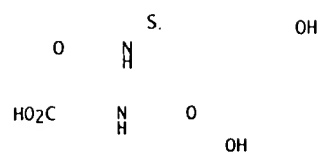
Absolute stereochemistry.



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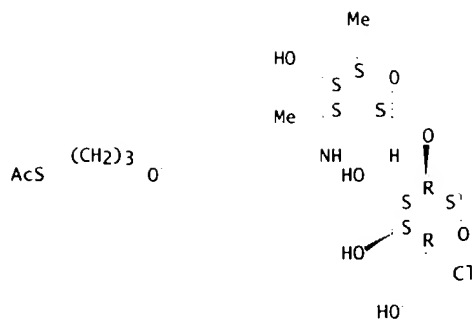
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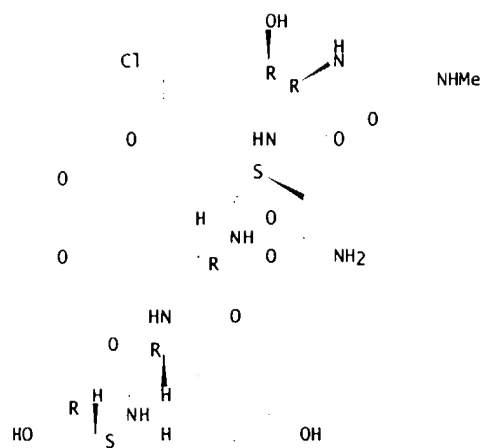
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NAME)

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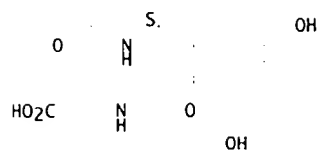
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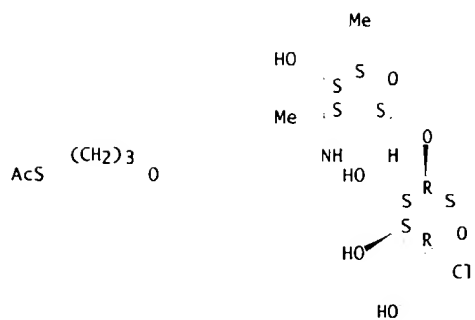


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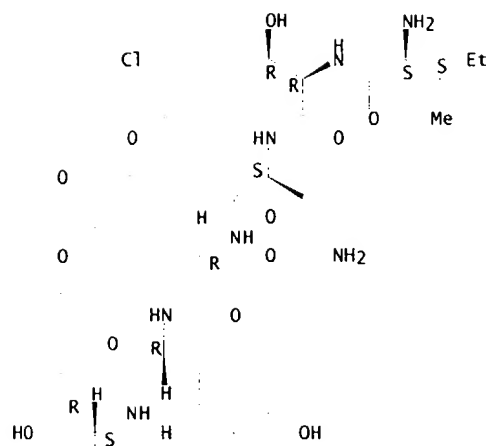
Absolute stereochemistry.



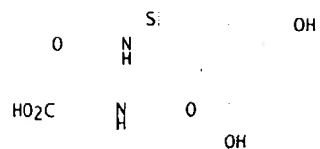
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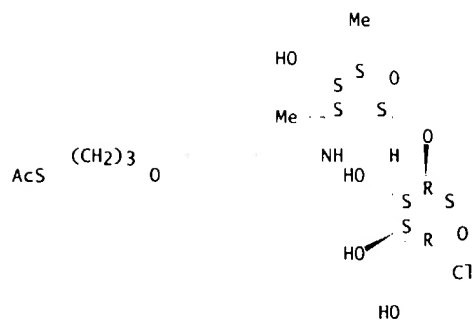
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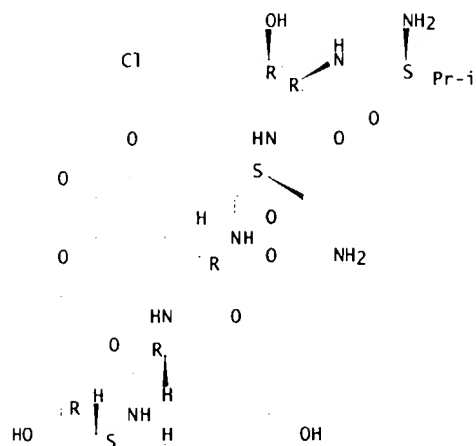
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Absolute stereochemistry.

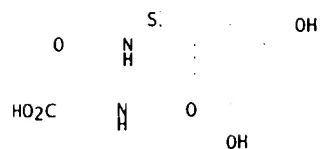
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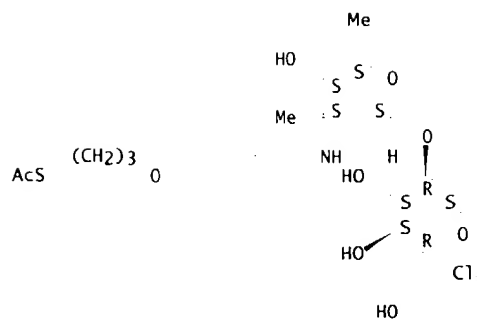
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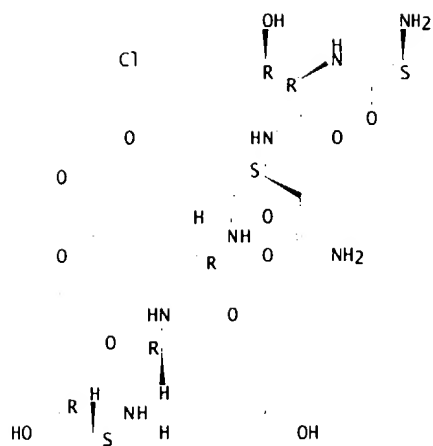
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Absolute stereochemistry.

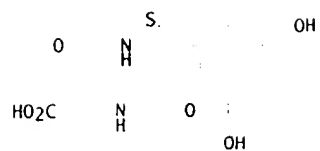
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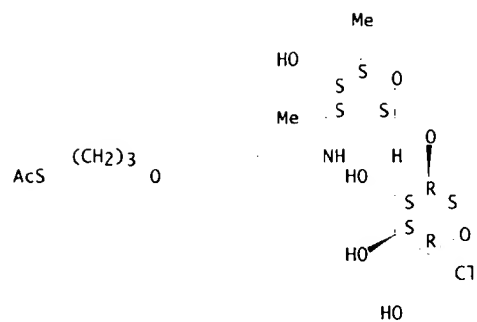
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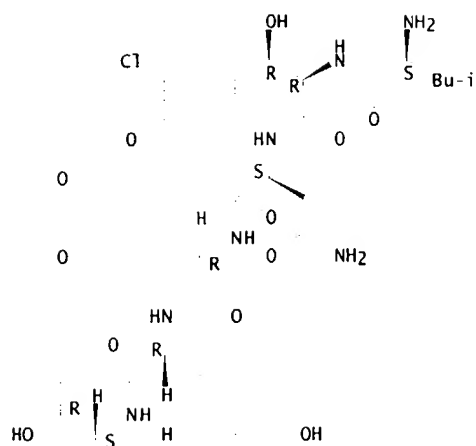
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 (CA INDEX NAME)

Absolute stereochemistry.

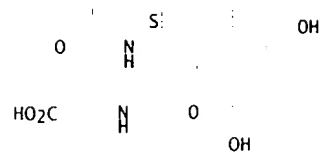
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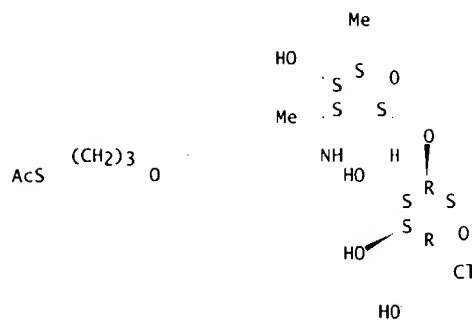
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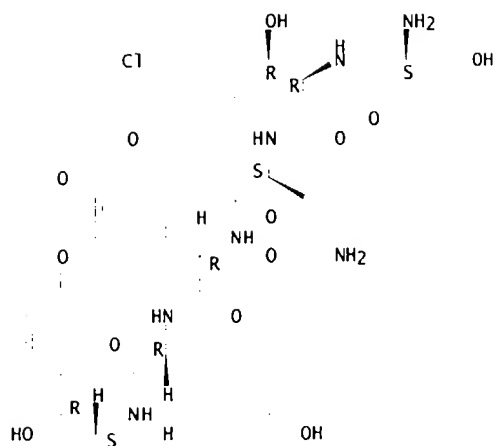
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Absolute stereochemistry.

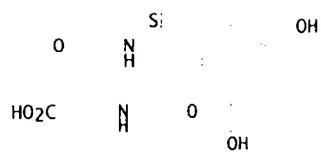
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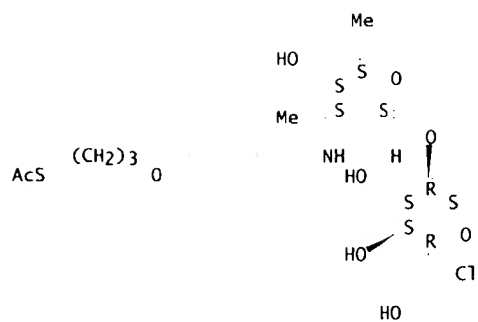
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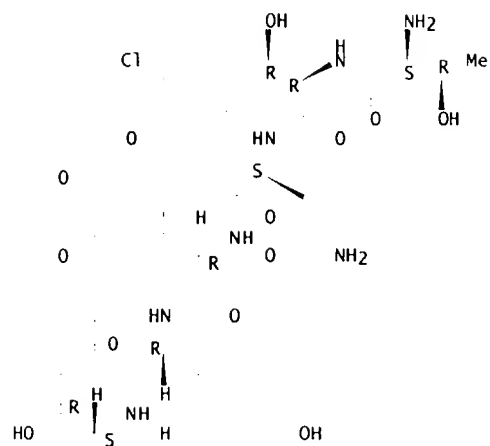
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Absolute stereochemistry.

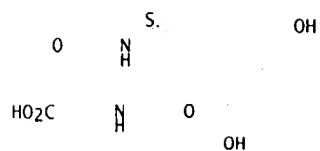
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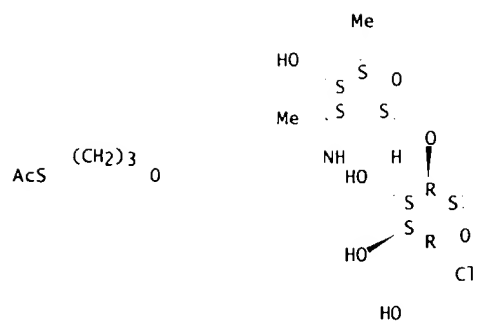
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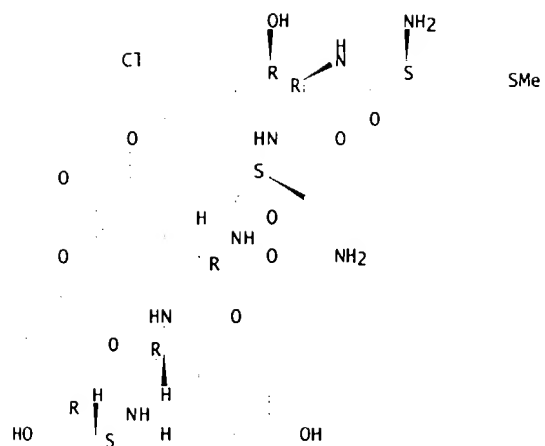
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Absolute stereochemistry.

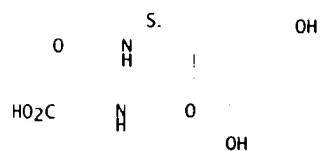
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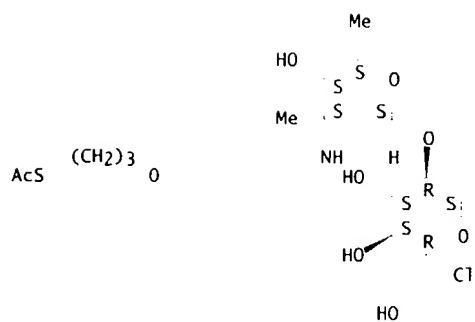
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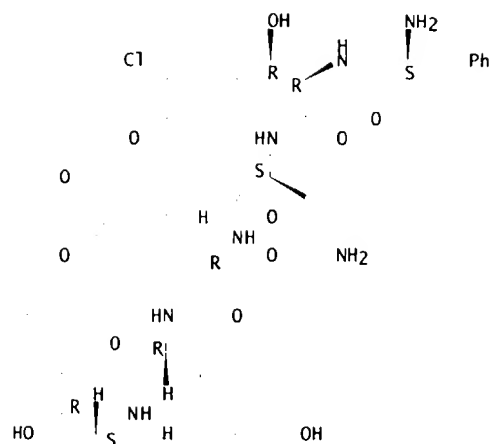
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Absolute stereochemistry.

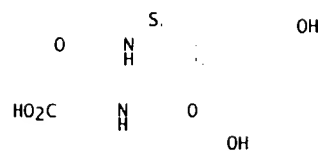
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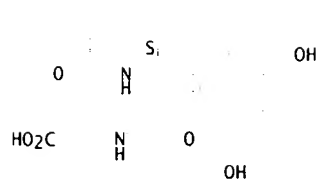
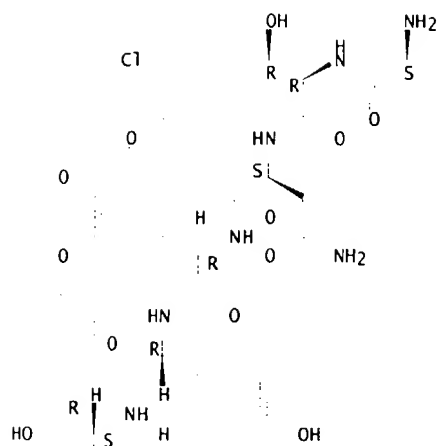


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Absolute stereochemistry.

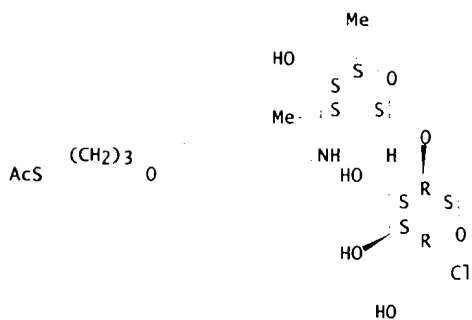




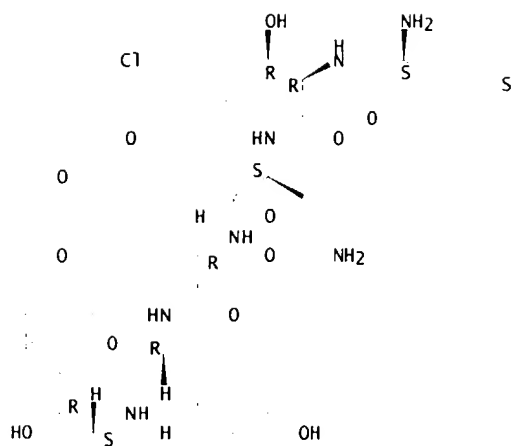
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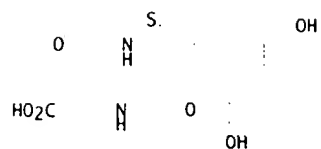
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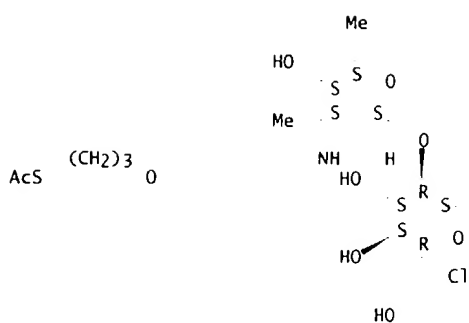
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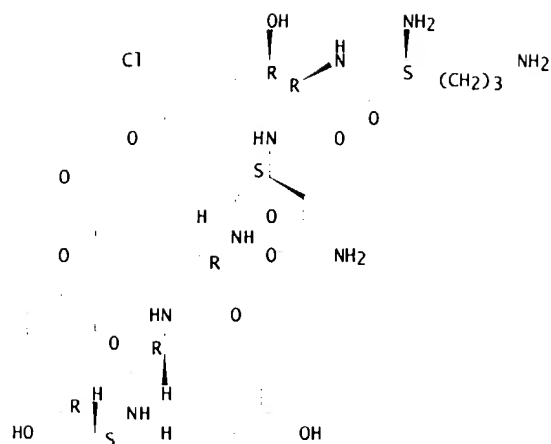
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 INDEX NAME)

Absolute stereochemistry.

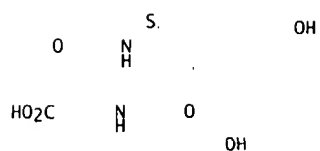
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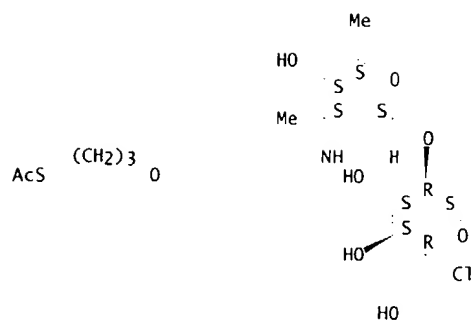
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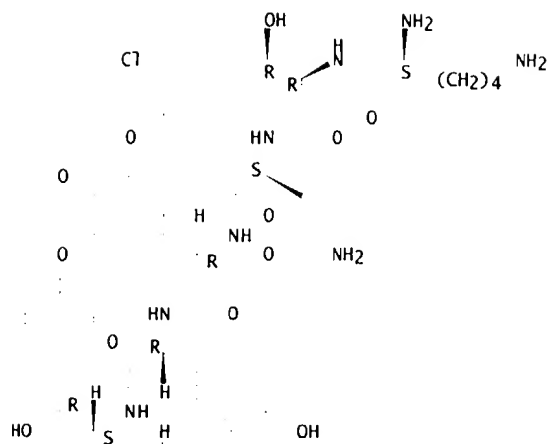
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 INDEX NAME)

Absolute stereochemistry.

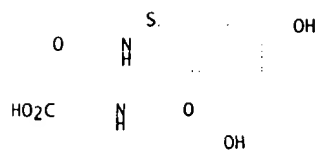
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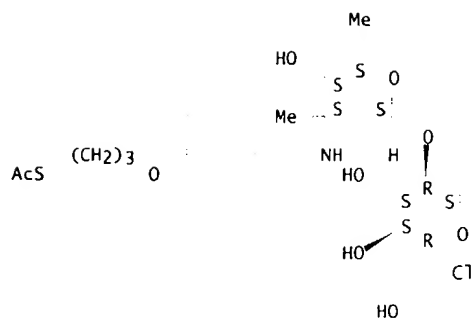
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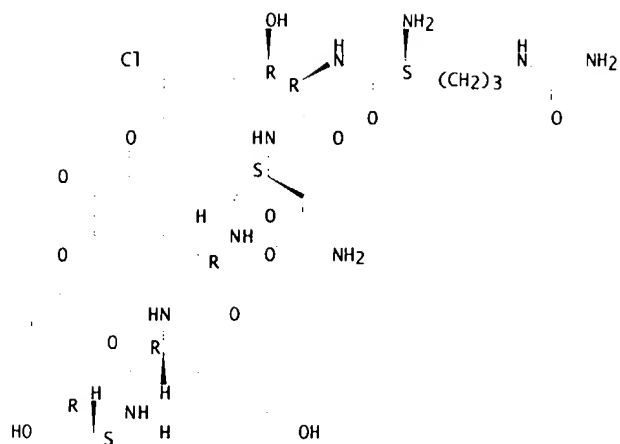
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Absolute stereochemistry.

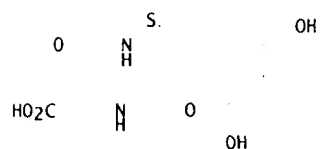
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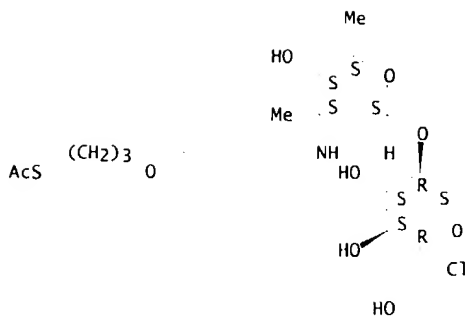
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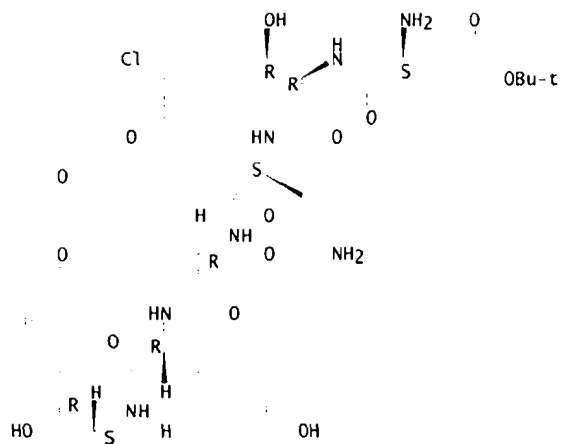
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Absolute stereochemistry.

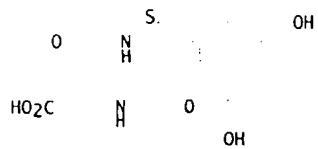
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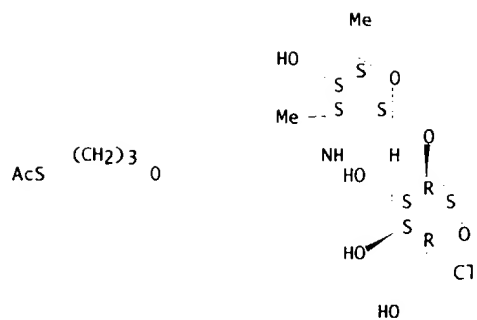


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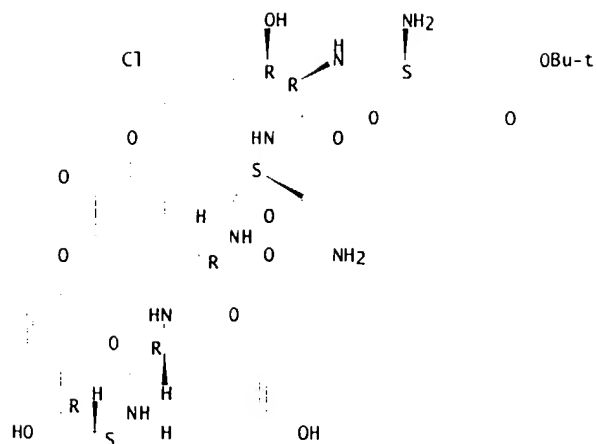
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**Absolute stereochemistry.**

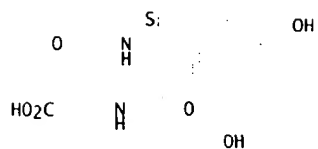
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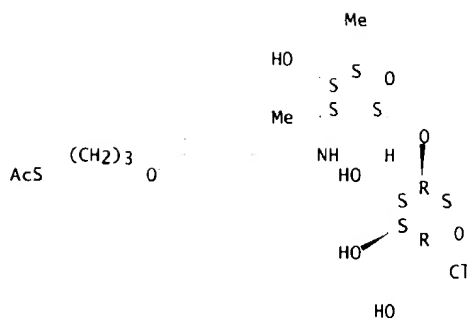
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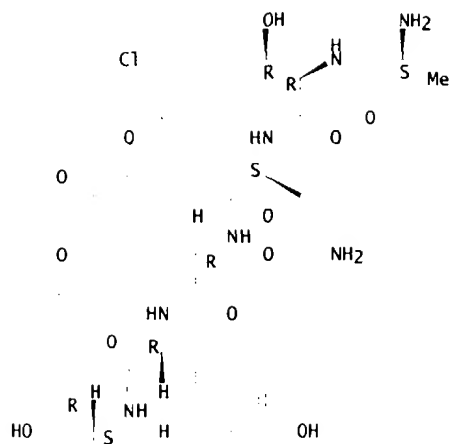
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Absolute stereochemistry.

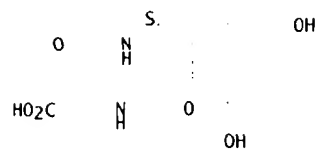
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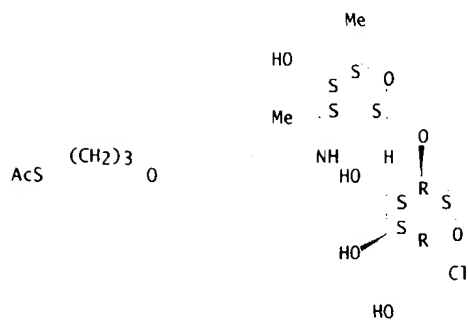


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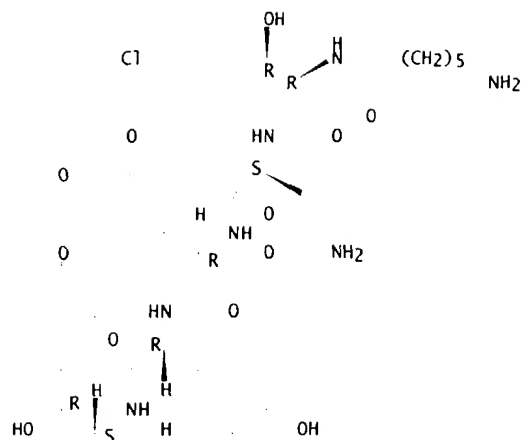
Absolute stereochemistry.



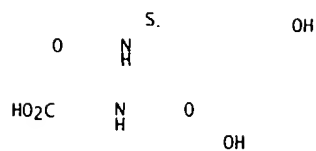
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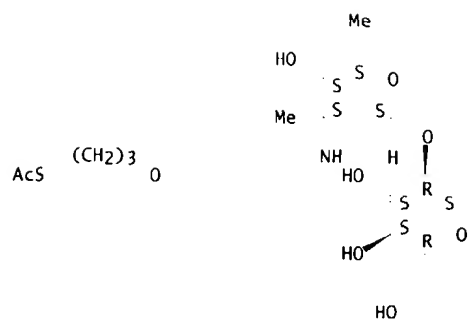
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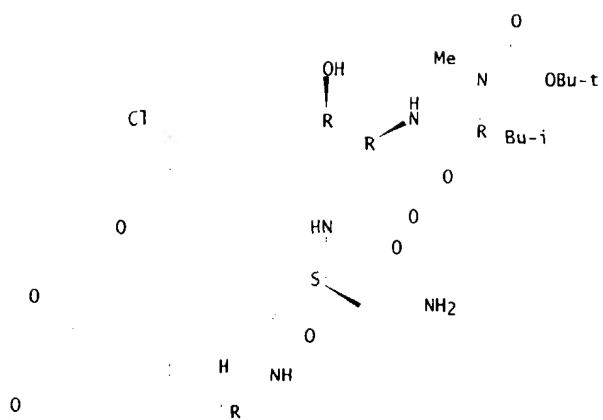
IT 383424-29-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)  
 RN 383424-29-1 CAPLUS  
 CN Vancomycin, N3''-[[[3-[3-(acetylthio)propoxy]phenyl]methyl]-56-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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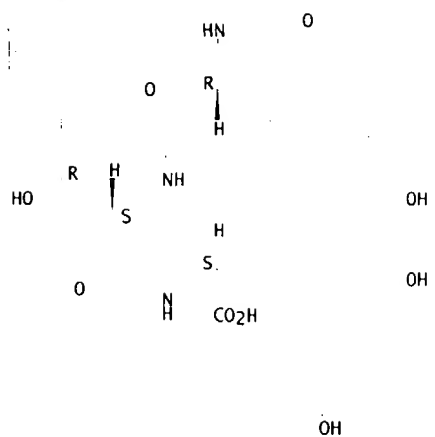
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IT 383424-30-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

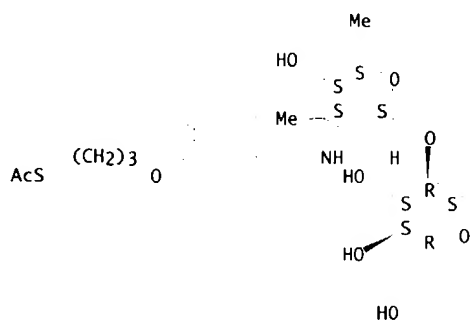
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)

RN 383424-30-4 CAPLUS

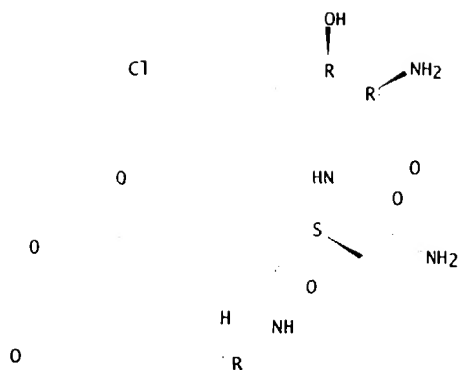
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Absolute stereochemistry.

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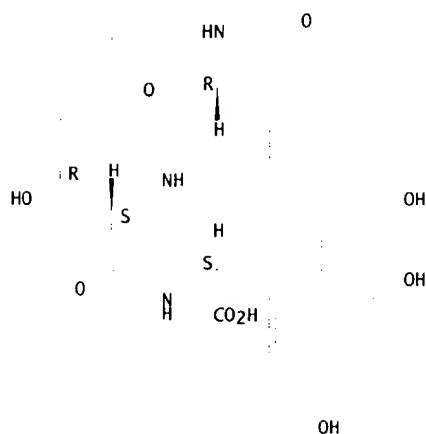
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REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2000:818978 CAPLUS

DOCUMENT NUMBER: 134:116215

TITLE: Target-accelerated combinatorial synthesis and discovery of highly potent antibiotics effective against vancomycin-resistant bacteria

AUTHOR(S): Nicolaou, K. C.; Hughes, Robert; Cho, Suk Young; Winssinger, Nicolas; Smethurst, Christian; Labischinski, Harald; Endermann, Rainer

CORPORATE SOURCE: Skaggs Inst. Chemical Biology, Scripps Res. Inst., La Jolla, CA, 92037, USA

SOURCE: Angewandte Chemie, International Edition (2000), 39(21), 3823-3828

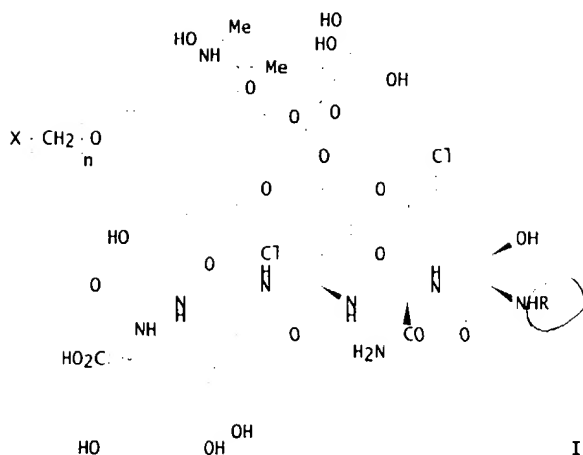
CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

Nov. 3 (2000)



AB The authors report the application of direct target-accelerated combinatorial synthesis (TACS) of vancomycin dimers for the identification of ligands with the highest affinity for vancomycin's receptor, D-Ala-D-Ala. For example, solid- and soln.-phase combinatorial chem. were used to synthesize a library of vancomycin substrates, from which a set of monomers I [n = 2-4; X = SCOMe, CH:CH2; R = H, D-(NMe)Leu, .beta.-Ala, L-Asn, etc.] were chosen for the target-accelerated dimerization step. I (X = SCOMe) was subjected to ligation by disulfide bond formation and I (X = CH:CH2) was subjected to ligation by olefin metathesis in both the absence and presence of vancomycin's targets, Ac-D-Ala-D-Ala-OH and Ac-Lys(Ac)-D-Ala-D-Ala-OH, for which vancomycin has the greatest affinity. Here, a strong target-induced rate acceleration was obsd. in the presence of these targets. Thus, target-accelerated combinatorial synthesis was performed, and from this library, several olefin metathesis dimers of I [n = 2-4; R = H, D-(NMe)Leu, .beta.-Ala, Asn] and disulfide dimers of I [n = 2,3; R = D-(NMe)Leu] were identified, and these were, then, individually synthesized from their resp. monomers. Antibacterial activity for these dimers were reported; of them, some have potent activities against vancomycin-resistant enterococci (VRE) and vancomycin intermediate susceptible *Staphylococcus aureus* (VISA) that rival or exceed the most active compds. known today for these bacterial strains.

IT 321362-15-6P 321362-17-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

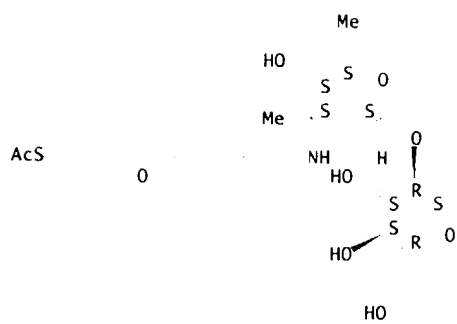
(prepn. of vancomycin substrates for the target-accelerated combinatorial synthesis of vancomycin dimers)

RN 321362-15-6 CAPLUS

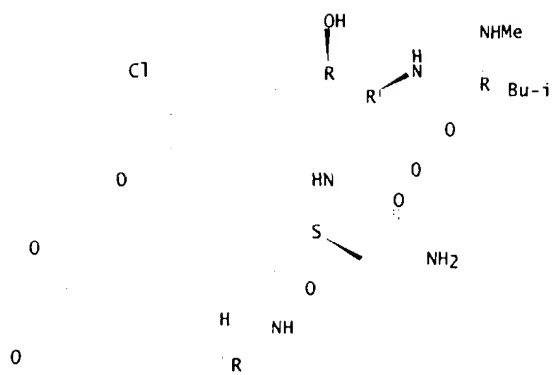
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**Absolute stereochemistry.**

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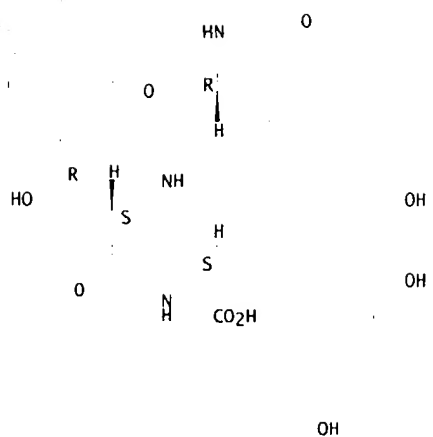
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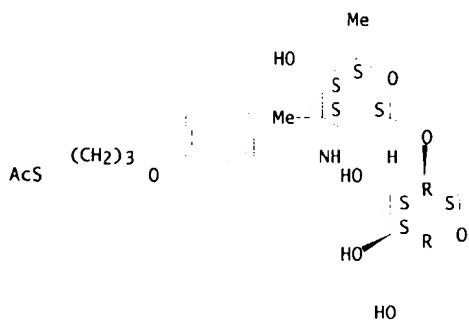
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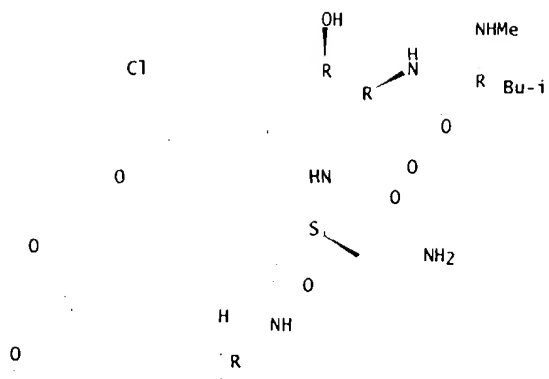
RN 321362-17-8 CAPLUS  
 CN Vancomycin, N3''-[3-[3-(acetylthio)propoxy]phenyl]methyl]- (9CI) (CA  
 INDEX NAME)

Absolute stereochemistry.

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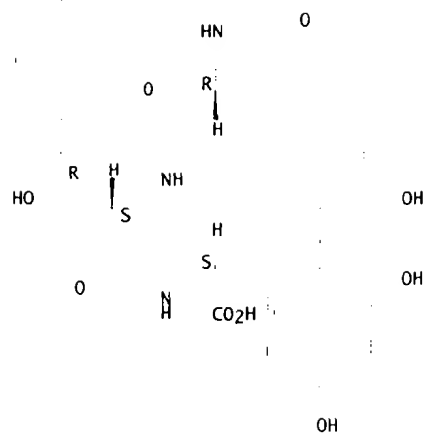
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36

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